

=> d his

(FILE 'HOME' ENTERED AT 13:54:39 ON 31 MAY 2011)

FILE 'REGISTRY' ENTERED AT 13:54:48 ON 31 MAY 2011

```
      E (104-45-0)/RN
      E (135-02-4)/RN
      E (151-10-0)/RN
      E DIHYDROANETHOLE/CN
L1      1 S E35
      E O-ANISALDEHYDE/CN
L2      1 S E47
      E 1,3-DIMETHOXYBENZENE/CN
L3      1 S E59
      E 2-HYDROXYACETOPHENONE/CN
L4      1 S E71
      E 2-METHOXYACETOPHENONE/CN
L5      1 S E83
```

FILE 'HOME' ENTERED AT 14:00:21 ON 31 MAY 2011

FILE 'STINGUIDE' ENTERED AT 14:13:17 ON 31 MAY 2011

FILE 'FOMAD, FROSTI, FSTA' ENTERED AT 14:19:56 ON 31 MAY 2011

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L6      0 S L1
L7      0 S L2
L8      0 S L3
L9      0 S L4
L10     0 S L5
L11     146 S METHYL SALICYLATE
L12     42 S P-ANISALDEHYDE
L13     3 S O-ANISALDEHYDE
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FILE 'MEDLINE, HCAPLUS' ENTERED AT 14:24:22 ON 31 MAY 2011

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L14     1505 S O-METHOXYBENZALDEHYDE OR O-ANISALDEHYDE
L15     3 S L14 (L) APPLE JUICE
L16     3 S L2 (L) APPLE JUICE
L17     0 S L15 NOT L16
L18     19 S L1 (S) (FLAVOR? OR AROMA OR ODOR? OR ODOUR? OR FLAVOUR?)
L19     15 S L2 (S) (FLAVOR? OR AROMA OR ODOR? OR ODOUR? OR FLAVOUR?)
L20     29 S L3 (S) (FLAVOR? OR AROMA OR ODOR? OR ODOUR? OR FLAVOUR?)
L21     6 S L4 (S) (FLAVOR? OR AROMA OR ODOR? OR ODOUR? OR FLAVOUR?)
L22     1 S L5 (S) (FLAVOR? OR AROMA OR ODOR? OR ODOUR? OR FLAVOUR?)
L23     1 S L22 AND PY<2004
L24     4 S L21 AND PY<2004
L25     12 S L20 AND PY<2004
L26     6 S L19 AND PY<2004
L27     10 S L18 AND PY<2004
L28     31 S L23 OR L24 OR L25 OR L26 OR L27
```

=> s l28 and (flavor? or flavour?)

L29 20 L28 AND (FLAVOR? OR FLAVOUR?)

=> d ibib iabs kwic hit 1-20

THE ESTIMATED COST FOR THIS REQUEST IS 72.00 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L29 ANSWER 1 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2003:791065 HCAPLUS

DOCUMENT NUMBER: 140:41025

TITLE: Truffle aroma characterization by headspace

AUTHOR(S): solid-phase microextraction  
CORPORATE SOURCE: Diaz, P.; Ibanez, E.; Senorans, F. J.; Reglero, G.  
SOURCE: Universidad Catolica de Avila, Avila, 05005, Spain  
Journal of Chromatography, A (2003), 1017(1-2),  
207-214

CODEN: JCRAEY; ISSN: 0021-9673  
Elsevier Science B.V.

PUBLISHER:  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
ABSTRACT:

In the present study, a headspace solid-phase microextraction (HS-SPME) combined to gas chromatography-mass spectrometry (GC-MS) was used to fully characterize aroma of truffles of different species. A fiber of medium polarity (for flavors) was used to avoid discrimination towards very non-polar and polar volatile compounds. In a previous work, extraction conditions were optimized by means of an experimental design leading to the following conditions that were used in the present study: extraction temperature, 53 °C; extraction time, 13.6 min; and equilibrium time, 5 min.

A comparison among different truffles species has been established in terms of qualitative and quantitative differences on volatile composition. By using the optimal extraction conditions and GC-MS it was possible to identify 89 compounds in 2 different truffle species such as *Tuber aestivum* and *Tuber melanosporum*. An attempt was made to be able to determine the influence of different geographical origins on the aroma fraction of such fungi.

SO Journal of Chromatography, A (2003), 1017(1-2), 207-214  
CODEN: JCRAEY; ISSN: 0021-9673

AB . . . chromatography-mass spectrometry (GC-MS) was used to fully characterize aroma of truffles of different species. A fiber of medium polarity (for flavors) was used to avoid discrimination towards very non-polar and polar volatile compounds. In a previous work, extraction conditions were optimized. . .

IT Flavor  
Odor and Odorous substances  
*Tuber aestivum*  
*Tuber melanosporum*  
Tuberaceae  
Volatile substances

(truffle aroma characterization by headspace solid-phase microextraction.)  
IT 60-12-8, Phenylethanol 64-19-7, Acetic acid, biological studies  
66-25-1, Hexanal 67-64-1, 2-Propanone, biological studies 67-68-5,  
Sulfinylbismethane, biological studies 75-07-0, Acetaldehyde, biological  
studies 75-18-3, Dimethyl sulfide 78-83-1, 2-Methyl-1-propanol,  
biological studies 78-92-2, 2-Butanol 78-93-3, 2-Butanone, biological  
studies 79-10-7, 2-Propenoic acid, biological studies 88-69-7,  
2-(1-Methylethyl)phenol 91-16-7, 1,2-Dimethoxybenzene 91-20-3,  
Naphthalene, biological studies 93-15-2,  
1,2-Dimethoxy-4-(2-propenyl)benzene 95-47-6, 1,2-Dimethylbenzene,  
biological studies 95-63-6, 1,2,4-Trimethylbenzene 96-17-3,  
2-Methylbutanal 96-48-0, 2(3H)-Dihydrofuranone 98-01-1,  
2-Furancarboxaldehyde, biological studies 100-41-4, Ethylbenzene,  
biological studies 100-52-7, Benzaldehyde, biological studies  
100-66-3, Methoxybenzene, biological studies 100-84-5,  
1-Methoxy-3-methylbenzene 104-46-1, 1-Methoxy-4-(1-propenyl)benzene  
104-76-7, 2-Ethyl-1-hexanol 106-42-3, 1,4-Dimethylbenzene, biological  
studies 106-44-5, p-Cresol, biological studies 106-68-3, 3-Octanone  
108-38-3, 1,3-Dimethylbenzene, biological studies 108-64-5, Ethyl  
3-methylbutanoate 108-88-3, Methylbenzene, biological studies  
108-95-2, Phenol, biological studies 111-13-7, 2-Octanone 111-27-3,  
1-Hexanol, biological studies 111-70-6, 1-Heptanol 111-71-7, Heptanal

112-12-9, 2-Undecanone 112-31-2, Decanal 112-54-9, Dodecanal  
 122-78-1, Phenylacetaldehyde 123-38-6, Propanal, biological studies  
 123-51-3, 3-Methyl-1-butanol 124-13-0, Octanal 124-19-6, Nonanal  
 128-37-0, 2,6-Bis(1,1-dimethylethyl)-4-methylphenol, biological studies  
 137-32-6, 2-Methyl-1-butanol 141-78-6, Ethyl acetate, biological studies  
 151-10-0, 1,3-Dimethoxybenzene 494-99-5, 3,4-Dimethoxytoluene  
 513-86-0, 3-Hydroxy-2-butanone 565-62-8, 3-Methyl-3-penten-2-one  
 585-25-1, 2,3-Octanedione 589-59-3, 2-Methylpropyl-3-methylbutanoate  
 589-98-0, 3-Octanol 590-86-3, 3-Methylbutanal 620-83-7,  
 1-Methyl-4-(phenylmethyl)benzene 624-92-0, Dimethyl disulfide  
 625-33-2, 3-Penten-2-one 1115-11-3, 2-Methyl-2-butenal 1453-58-3  
 1481-93-2, 4-Hydroxychroman 1669-44-9, 3-Octen-2-one 1758-88-9,  
 2-Ethyl-1,4-dimethylbenzene 2050-01-3, 3-Methylbutyl-2-methylpropanoate  
 2363-88-4, 2,4-Decadienal 2363-89-5, 2-Octenal 2445-67-2 2445-78-5,  
 2-Methylbutyl-2-methylbutanoate 2463-63-0, 2-Heptenal 3391-86-4,  
 1-Octen-3-ol 3658-80-8, Dimethyl trisulfide 3777-69-3, 2-Pentylfuran  
 4170-30-3, 2-Butenal 4411-89-6 4536-23-6, 2-Methylhexanoic acid  
 5920-29-6 6750-03-4, 2,4-Nonadienal 6836-38-0, 6-Dodecanol  
 14044-41-8 15706-73-7, Butyl 2-methylbutanoate 18217-12-4,  
 5-Methyl-2-heptanone 19872-52-7, 4-Mercapto-4-methyl-2-pentanone  
 24599-58-4, 2,5-Dimethoxytoluene 25415-62-7, Pentyl 3-methylbutanoate  
 34314-83-5, 2,3-Dihydro-4-methylfuran 83861-74-9, Octa-1,5-dien-3-ol  
 120550-70-1

RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)  
 (truffle aroma characterization by headspace solid-phase microextrn.)

OS.CITING REF COUNT: 34 THERE ARE 34 CAPLUS RECORDS THAT CITE THIS RECORD (34 CITINGS)  
 REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT  
 SO Journal of Chromatography, A (2003), 1017(1-2), 207-214  
 CODEN: JCRAEY; ISSN: 0021-9673

AB In the present study, a headspace solid-phase microextrn. (HS-SPME) combined to gas chromatog.-mass spectrometry (GC-MS) was used to fully characterize aroma of truffles of different species. A fiber of medium polarity (for flavors) was used to avoid discrimination towards very non-polar and polar volatile compds. In a previous work, extraction conditions were optimized by means of an exptl. design leading to the following conditions that were used in the present study: extraction temperature, 53 °C; extraction time, 13.6 min; and equilibrium time, 5 min. A comparison among different truffles species has been established in terms of qual. and quant. differences on volatile composition. By using the optimal extraction conditions and GC-MS it was possible to identify 89 compds. in 2 different truffle species such as Tuber aestivum and Tuber melanosporum. An attempt was made to be able to determine the influence of different geog. origins on the aroma fraction of such fungi.

IT Flavor  
 Odor and Odorous substances  
 Tuber aestivum  
 Tuber melanosporum  
 Tuberaceae  
 Volatile substances  
 (truffle aroma characterization by headspace solid-phase microextrn.)

IT 60-12-8, Phenylethanol 64-19-7, Acetic acid, biological studies  
 66-25-1, Hexanal 67-64-1, 2-Propanone, biological studies 67-68-5,  
 Sulfinylbismethane, biological studies 75-07-0, Acetaldehyde, biological studies 75-18-3, Dimethyl sulfide 78-83-1, 2-Methyl-1-propanol, biological studies 78-92-2, 2-Butanol 78-93-3, 2-Butanone, biological studies 79-10-7, 2-Propenoic acid, biological studies 88-69-7,  
 2-(1-Methylethyl)phenol 91-16-7, 1,2-Dimethoxybenzene 91-20-3,

Naphthalene, biological studies 93-15-2,  
 1,2-Dimethoxy-4-(2-propenyl)benzene 95-47-6, 1,2-Dimethylbenzene,  
 biological studies 95-63-6, 1,2,4-Trimethylbenzene 96-17-3,  
 2-Methylbutanal 96-48-0, 2(3H)-Dihydrofuranone 98-01-1,  
 2-Furancarboxaldehyde, biological studies 100-41-4, Ethylbenzene,  
 biological studies 100-52-7, Benzaldehyde, biological studies  
 100-66-3, Methoxybenzene, biological studies 100-84-5,  
 1-Methoxy-3-methylbenzene 104-46-1, 1-Methoxy-4-(1-propenyl)benzene  
 104-76-7, 2-Ethyl-1-hexanol 106-42-3, 1,4-Dimethylbenzene, biological  
 studies 106-44-5, p-Cresol, biological studies 106-68-3, 3-Octanone  
 108-38-3, 1,3-Dimethylbenzene, biological studies 108-64-5, Ethyl  
 3-methylbutanoate 108-88-3, Methylbenzene, biological studies  
 108-95-2, Phenol, biological studies 111-13-7, 2-Octanone 111-27-3,  
 1-Hexanol, biological studies 111-70-6, 1-Heptanol 111-71-7, Heptanal  
 112-12-9, 2-Undecanone 112-31-2, Decanal 112-54-9, Dodecanal  
 122-78-1, Phenylacetaldehyde 123-38-6, Propanal, biological studies  
 123-51-3, 3-Methyl-1-butanol 124-13-0, Octanal 124-19-6, Nonanal  
 128-37-0, 2,6-Bis(1,1-dimethylethyl)-4-methylphenol, biological studies  
 137-32-6, 2-Methyl-1-butanol 141-78-6, Ethyl acetate, biological studies  
 151-10-0, 1,3-Dimethoxybenzene 494-99-5, 3,4-Dimethoxytoluene  
 513-86-0, 3-Hydroxy-2-butanone 565-62-8, 3-Methyl-3-penten-2-one  
 585-25-1, 2,3-Octanedione 589-59-3, 2-Methylpropyl-3-methylbutanoate  
 589-98-0, 3-Octanol 590-86-3, 3-Methylbutanal 620-83-7,  
 1-Methyl-4-(phenylmethyl)benzene 624-92-0, Dimethyl disulfide  
 625-33-2, 3-Penten-2-one 1115-11-3, 2-Methyl-2-butanal 1453-58-3  
 1481-93-2, 4-Hydroxychroman 1669-44-9, 3-Octen-2-one 1758-88-9,  
 2-Ethyl-1,4-dimethylbenzene 2050-01-3, 3-Methylbutyl-2-methylpropanoate  
 2363-88-4, 2,4-Decadienal 2363-89-5, 2-Octenal 2445-67-2 2445-78-5,  
 2-Methylbutyl-2-methylbutanoate 2463-63-0, 2-Heptenal 3391-86-4,  
 1-Octen-3-ol 3658-80-8, Dimethyl trisulfide 3777-69-3, 2-Pentylfuran  
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 14044-41-8 15706-73-7, Butyl 2-methylbutanoate 18217-12-4,  
 5-Methyl-2-heptanone 19872-52-7, 4-Mercapto-4-methyl-2-pentanone  
 24599-58-4, 2,5-Dimethoxytoluene 25415-62-7, Pentyl 3-methylbutanoate  
 34314-83-5, 2,3-Dihydro-4-methylfuran 83861-74-9, Octa-1,5-dien-3-ol  
 120550-70-1  
 RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical  
 study); BIOL (Biological study)  
 (truffle aroma characterization by headspace solid-phase  
 microextn.)

L29 ANSWER 2 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2003:230629 HCAPLUS

DOCUMENT NUMBER: 138:384323

TITLE: Investigation of beer flavor by gas chromatography-olfactometry

AUTHOR(S): Murakami, A. A.; Goldstein, H.; Navarro, A.; Seabrooks, J. R.; Ryder, D. S.

CORPORATE SOURCE: Miller Brewing Company, Milwaukee, WI, 53201, USA  
 SOURCE: Journal of the American Society of Brewing Chemists (2003), 61(1), 23-32  
 CODEN: JSBCD3; ISSN: 0361-0470

PUBLISHER: American Society of Brewing Chemists, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

ABSTRACT:

Gas chromatog.-olfactometry (GC-O) is an anal. technique for evaluating the aroma characteristics of volatile constituents separated by gas chromatog. (GC). This article presents 3 case studies employing the GC-O technique in brewing, including investigation of kettle hop aroma, an off-aroma in beer, and

aged-beer aroma. The kettle hop aroma was studied using a GC-O technique called CharmAnal. (DATU, Inc., Geneva, NY) and beer strongly hopped with Oregon Cascade hop pellets at 45 min before end of kettle boil. CharmAnal. can quantitate the intensity of an aroma detected at a sniff port. It revealed that linalool was an important aroma compound in hopped beer and that phenylethyl alc. and two Co-eluting, tentatively identified constituents were important aroma compds. in hopped and unhopped beers. In a second study, GC-O was employed for investigating an objectionable aroma described as medicinal/phenolic/Band-Aid in a production beer. GC-O was able to reveal the eluting off-odor that matched the off-aroma character in the beer. In a third case study, a quant. GC-O technique called AromaTrax (Microanalytics, Round Rock, TX) was employed to determine aged-beer aroma. This technique revealed that quant. changes of many minor components possessing unpleasant aroma notes, particularly the carboxylic acids, were involved in aged-beer aroma.

TI Investigation of beer flavor by gas chromatography-olfactometry  
 SO Journal of the American Society of Brewing Chemists (2003), 61(1), 23-32  
 CODEN: JSBCD3; ISSN: 0361-0470  
 ST beer flavor detection gas chromatog olfactometry  
 IT Brewing  
 Gas chromatography  
 Humulus  
 Odor and Odorous substances  
 Volatile substances  
 (beer flavor by gas chromatog.-olfactometry)  
 IT Beer analysis  
 (beer flavor by gas chromatog.-olfactometry in)  
 IT Odor and Odorous substances  
 (off-odor; beer flavor by gas chromatog.-olfactometry)  
 IT 60-12-8, Phenylethyl alcohol 71-41-0, Amyl alcohol, biological studies  
 78-70-6, Linalool 97-62-1, Ethyl 2-methylpropanoate 98-00-0,  
 2-Furanmethanol 103-36-6, Ethyl cinnamate 103-45-7, 2-Phenylethyl  
 acetate 104-67-6,  $\gamma$ -Undecalactone 105-54-4, Ethyl butyrate  
 106-24-1, trans-Geraniol 106-25-2, Nerol 110-38-3, Ethyl decanoate  
 118-71-8, Maltol 121-33-5, Vanillin 123-51-3, 3-Methyl-1-butanol  
 123-66-0, Ethyl hexanoate 123-92-2, Isoamyl acetate 503-74-2,  
 3-Methylbutyric acid 527-35-5, 2,3,5,6-Tetramethylphenol 551-93-9,  
 o-Aminoacetophenone 934-34-9, 2-(3H)-Benzothiazolone 1450-72-2,  
 1-(2-Hydroxy-5-methylphenyl)ethanone 3658-80-8, Dimethyl trisulfide  
 4079-52-1, 2-Methoxyacetophenone 6617-49-8 7786-61-0,  
 4-Vinylguaiacol 23726-93-4,  $\beta$ -Damascenone  
 RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical  
 study); BIOL (Biological study)  
 (beer flavor by gas chromatog.-olfactometry)  
 OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS  
 RECORD (11 CITINGS)  
 REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT  
 TI Investigation of beer flavor by gas chromatography-olfactometry  
 SO Journal of the American Society of Brewing Chemists (2003), 61(1), 23-32  
 CODEN: JSBCD3; ISSN: 0361-0470  
 ST beer flavor detection gas chromatog olfactometry  
 IT Brewing  
 Gas chromatography  
 Humulus  
 Odor and Odorous substances  
 Volatile substances  
 (beer flavor by gas chromatog.-olfactometry)  
 IT Beer analysis  
 (beer flavor by gas chromatog.-olfactometry in)  
 IT Odor and Odorous substances

(off-odor; beer flavor by gas chromatog.-olfactometry)

IT 60-12-8, Phenylethyl alcohol 71-41-0, Amyl alcohol, biological studies  
 78-70-6, Linalool 97-62-1, Ethyl 2-methylpropanoate 98-00-0,  
 2-Furanmethanol 103-36-6, Ethyl cinnamate 103-45-7, 2-Phenylethyl  
 acetate 104-67-6,  $\gamma$ -Undecalactone 105-54-4, Ethyl butyrate  
 106-24-1, trans-Geraniol 106-25-2, Nerol 110-38-3, Ethyl decanoate  
 118-71-8, Maltol 121-33-5, Vanillin 123-51-3, 3-Methyl-1-butanol  
 123-66-0, Ethyl hexanoate 123-92-2, Isoamyl acetate 503-74-2,  
 3-Methylbutyric acid 527-35-5, 2,3,5,6-Tetramethylphenol 551-93-9,  
 o-Aminoacetophenone 934-34-9, 2-(3H)-Benzothiazolone 1450-72-2,  
 1-(2-Hydroxy-5-methylphenyl)ethanone 3658-80-8, Dimethyl trisulfide  
 4079-52-1, 2-Methoxyacetophenone 6617-49-8 7786-61-0,  
 4-Vinylguaiacol 23726-93-4,  $\beta$ -Damascenone  
 RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical  
 study); BIOL (Biological study)  
 (beer flavor by gas chromatog.-olfactometry)

L29 ANSWER 3 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2001:912026 HCAPLUS

DOCUMENT NUMBER: 136:324259

TITLE: Headspace aroma of "wild onion" trees

AUTHOR(S): Yang, Xiaogen; Josephson, Dave; Peppet, Jeff;  
 Eilerman, Robert; Grab, Willi; Gassenmeier, Klaus  
 CORPORATE SOURCE: Givaudan Flavors Corp., Cincinnati, OH, 45216, USA  
 SOURCE: Special Publication - Royal Society of Chemistry  
 (2001), 274(Food Flavors and Chemistry), 266-273  
 CODEN: SROCDQ; ISSN: 0260-6291

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

ABSTRACT:

In the Gabonese rain forest, there are at least 4 types of trees whose bark have strong garlic-like or onion-like odor. They are often called "wild onion trees". These trees were identified as *Afrostryax kamerunensis* Huac., *Scorodophloeus zenkere* Huac., *Hua gabonii* Huac., and *Afrostryax lepidophylleus* Huac. The bark of the trees are used for cooking. The leaves and seeds of *H. gabonii* and *A. lepidophylleus*, and the roots from young trees of *A. kamerunensis* are also used in flavoring sauces. In addition, the bark also are used for medicinal purposes. The volatile components of freshly cut bark of 3 species: *A. kamerunensis*, *S. zenkere*, *H. gabonii* were collected and analyzed. Many sulfur-containing compds. were present in the headspace. The character impact compds. were identified as di-Me disulfide, 2,3,5-trithiahexane, 2,4,6-trithiaheptane, and 2,4-dithiapentane by GC sniffing.

SO Special Publication - Royal Society of Chemistry (2001), 274(Food  
 Flavors and Chemistry), 266-273  
 CODEN: SROCDQ; ISSN: 0260-6291

AB . . . seeds of *H. gabonii* and *A. lepidophylleus*, and the roots from  
 young trees of *A. kamerunensis* are also used in flavoring sauces. In  
 addition, the bark also are used for medicinal purposes. The volatile  
 components of freshly cut bark of 3. . .

IT 60-12-8, Phenylethyl alcohol 64-17-5, Ethanol, biological studies  
 64-19-7, Acetic acid, biological studies 65-85-0, Benzoic acid,  
 biological studies 66-25-1, n-Hexanal 67-68-5, Dimethyl sulfoxide,  
 biological studies 67-71-0, Dimethyl sulfone 68-11-1, Mercaptoacetic  
 acid, biological studies 71-36-3, Butan-1-ol, biological studies  
 71-41-0, Amyl alcohol, biological studies 74-93-1, Methanethiol,  
 biological studies 78-93-3, Methyl ethyl ketone, biological studies  
 80-56-8,  $\alpha$ -Pinene 87-20-7, Iso-Amyl salicylate 87-44-5,  
 $\beta$ -Caryophyllene 88-84-6,  $\beta$ -Guaiene 91-57-6,  
 2-Methylnaphthalene 95-16-9, Benzothiazole 98-01-1, Furfural,

biological studies 98-86-2, Acetophenone, biological studies 99-85-4,  
 $\gamma$ -Terpinene 99-87-6, p-Cymene 100-47-0, Benzonitrile, biological  
 studies 100-51-6, Benzyl alcohol, biological studies 100-52-7,  
 Benzaldehyde, biological studies 100-66-3, Anisole, biological studies  
 104-76-7, 2-Ethylhexan-1-ol 106-21-8, 3,7-Dimethyl-1-octanol 106-68-3,  
 3-Octanone 107-89-1, 3-Hydroxybutanal 107-92-6, n-Butyric acid,  
 biological studies 107-93-7, trans-2-Butenoic acid 108-95-2, Phenol,  
 biological studies 110-93-0, 6-Methylhept-5-en-2-one 111-27-3,  
 1-Hexanol, biological studies 111-71-7, Heptanal 112-05-0, Nonanoic  
 acid 112-32-3, n-Octyl formate 112-88-9, 1-Octadecene 112-92-5,  
 Octadecanol 118-56-9, Homomenthyl salicylate 118-60-5, 2-Ethylhexyl  
 salicylate 119-61-9, Benzophenone, biological studies 122-00-9,  
 p-Methylacetophenone 122-78-1, Phenyl acetaldehyde 123-35-3, Myrcene  
 123-42-2, 4-Hydroxy-4-methyl-2-pentanone 123-51-3, Iso-Amyl alcohol  
 123-72-8, Butanal 124-07-2, Octanoic acid, biological studies  
 124-13-0, Octanal 124-19-6, Nonanal 126-33-0, Tetrahydrothiophene,  
 1,1,dioxide 127-91-3,  $\beta$ -Pinene 128-37-0, Ionol, biological  
 studies 137-32-6, 2-Methylbutan-1-ol 138-86-3, Limonene 142-62-1,  
 Caproic acid, biological studies 142-91-6, Isopropyl palmitate  
 149-57-5, 2-Ethylhexanoic acid 289-16-7, 1,2,4-Trithiolane 291-22-5,  
 1,2,4,5-Tetrathiane 292-45-5, 1,2,4,6-Tetrathiepane 470-82-6,  
 1,8-Cineole 473-13-2,  $\alpha$ -Selinene 483-76-1,  $\delta$ -Cadinene  
 483-78-3, Cadalene 502-61-4, Farnesene 506-42-3,  
 trans-9-Octadecen-1-ol 512-61-8, Santalene 513-86-0, Acetoin  
 514-51-2,  $\beta$ -Patchoulene 536-74-3, Phenylacetylene 541-85-5,  
 5-Methyl-3-heptanone 555-10-2,  $\beta$ -Phellandrene 579-07-7,  
 1-Phenyl-1,2-propanedione 582-24-1,  
 $\alpha$ -Hydroxyacetophenone 586-62-9, Terpinolene 589-82-2, 3-Heptanol  
 589-98-0, Octan-3-ol 616-25-1, Pent-1-en-3-ol 617-94-7,  
 $\alpha$ , $\alpha$ -Dimethylbenzenemethanol 623-36-9 624-92-0, Dimethyl  
 disulfide 625-28-5, 3-Methyl butanenitrile 644-30-4,  $\alpha$ -Curcumene  
 732-26-3, Tri-tert-butyl phenol 926-37-4, 4,4-Dimethylpent-2-enal  
 928-96-1, cis-Hex-3-en-1-ol 930-60-9, 2-Cyclopentene-1,4-dione  
 933-48-2, Trioxal 1454-85-9, 1-Heptadecanol 1576-95-0, cis-2-Pentenol  
 1618-26-4, 2,4-Dithiapentane 1620-98-0,  
 3,5-Di-tert-butyl-4-hydroxybenzaldehyde 1741-83-9, 2-Thiaheptane  
 1795-15-9, Octylcyclohexane 1879-07-8, cis-p-Menth-8-ene 1879-09-0,  
 6-tert-Butyl-2,4-dimethyl phenol 2277-20-5, 6-Nonenal, (E)- 2314-48-9,  
 Carbonotrithiic acid dimethyl ester 2436-90-0, Citronellene  
 3338-55-4, cis- $\beta$ -Ocimene 3387-41-5, Sabinene 3391-86-4,  
 1-Octen-3-ol 3491-57-4 3592-19-6 3658-80-8, Dimethyl trisulfide  
 3777-69-3, 2-Pentylfuran 3913-02-8, 2-Butyl octanol 4130-42-1,  
 2,6-Bis(1,1-dimethylethyl)-4-ethylphenol 4170-30-3, 2-Butenal  
 4312-99-6, 1-Octen-3-one 4630-07-3, Valencene 4829-04-3,  
 1,3-Dithiolane 5008-72-0 5418-86-0 6540-86-9, 2,4,6-Trithiaheptane  
 6617-49-8 6728-26-3, trans-Hex-2-en-1-ol 6753-98-6, Humulene  
 6938-51-8, 2-Octylbenzoate 10522-26-6, 2-Methyl-1-undecanol 13877-93-5  
 15193-25-6, o-Menth-8-ene 16225-26-6, 3,5-Di-tert-butylbenzoic acid  
 16630-52-7, 3-Methylthiobutanol 17066-67-0,  $\beta$ -Selinene  
 17283-81-7, Dihydro  $\beta$ -ionone 17699-14-8,  $\alpha$ -Cubebene  
 18794-84-8, Trans- $\beta$ -Farnesene 19780-25-7, 2-Ethyl-2-butenal  
 20068-02-4 23986-74-5, Germacrene D 27070-58-2, Octadecene  
 27251-68-9, Pentadecene 27625-35-0, 3-Methylbutyl 2-methylbutyrate  
 33577-16-1 38514-13-5, 3-Ethyl-4-methyl-1-pentanol 38634-59-2,  
 Methylthiomethyl acetyl sulfide 42474-44-2, 2,3,5-Trithiahexane  
 51154-96-2, Massoialactone 58809-73-7, 2-Methylthiopropionic acid  
 66537-39-1 66537-40-4 80466-34-8, 2,4-Hexadienal 85544-38-3,  
 2,4,5,7-Tetrathiaoctane 103240-92-2 117210-66-9 119117-00-9  
 415686-96-3 415687-00-2

RL: ANT (Analyte); BSU (Biological study, unclassified); OCU (Occurrence,  
 unclassified); ANST (Analytical study); BIOL (Biological study); OCCU

(Occurrence)

(headspace aroma of wild onion trees)

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD  
(2 CITINGS)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

SO Special Publication - Royal Society of Chemistry (2001), 274(Food  
Flavors and Chemistry), 266-273  
CODEN: SROCDQ; ISSN: 0260-6291

AB In the Gabonese rain forest, there are at least 4 types of trees whose  
bark have strong garlic-like or onion-like odor. They are often called  
"wild onion trees". These trees were identified as *Afrostryax*  
*kamerunensis* Huac., *Scorodophloeus zenkerei* Huac., *Hua gabonii* Huac., and  
*Afrostryax lepidophyllus* Huac. The bark of the trees are used for  
cooking. The leaves and seeds of *H. gabonii* and *A. lepidophyllus*, and  
the roots from young trees of *A. kamerunensis* are also used in flavoring  
sauces. In addition, the bark also are used for medicinal purposes. The  
volatile components of freshly cut bark of 3 species: *A. kamerunensis*, *S.*  
*zenkerei*, *H. gabonii* were collected and analyzed. Many sulfur-containing  
comps. were present in the headspace. The character impact comps. were  
identified as di-Me disulfide, 2,3,5-trithiahexane, 2,4,6-trithiaheptane,  
and 2,4-dithiapentane by GC sniffing.

IT 60-12-8, Phenylethyl alcohol 64-17-5, Ethanol, biological studies  
64-19-7, Acetic acid, biological studies 65-85-0, Benzoic acid,  
biological studies 66-25-1, n-Hexanal 67-68-5, Dimethyl sulfoxide,  
biological studies 67-71-0, Dimethyl sulfone 68-11-1, Mercaptoacetic  
acid, biological studies 71-36-3, Butan-1-ol, biological studies  
71-41-0, Amyl alcohol, biological studies 74-93-1, Methanethiol,  
biological studies 78-93-3, Methyl ethyl ketone, biological studies  
80-56-8,  $\alpha$ -Pinene 87-20-7, Iso-Amyl salicylate 87-44-5,  
 $\beta$ -Caryophyllene 88-84-6,  $\beta$ -Guaiene 91-57-6,  
2-Methylnaphthalene 95-16-9, Benzothiazole 98-01-1, Furfural,  
biological studies 98-86-2, Acetophenone, biological studies 99-85-4,  
 $\gamma$ -Terpinene 99-87-6, p-Cymene 100-47-0, Benzonitrile, biological  
studies 100-51-6, Benzyl alcohol, biological studies 100-52-7,  
Benzaldehyde, biological studies 100-66-3, Anisole, biological studies  
104-76-7, 2-Ethylhexan-1-ol 106-21-8, 3,7-Dimethyl-1-octanol 106-68-3,  
3-Octanone 107-89-1, 3-Hydroxybutanal 107-92-6, n-Butyric acid,  
biological studies 107-93-7, trans-2-Butenoic acid 108-95-2, Phenol,  
biological studies 110-93-0, 6-Methylhept-5-en-2-one 111-27-3,  
1-Hexanol, biological studies 111-71-7, Heptanal 112-05-0, Nonanoic  
acid 112-32-3, n-Octyl formate 112-88-9, 1-Octadecene 112-92-5,  
Octadecanol 118-56-9, Homomenthyl salicylate 118-60-5, 2-Ethylhexyl  
salicylate 119-61-9, Benzophenone, biological studies 122-00-9,  
p-Methylacetophenone 122-78-1, Phenyl acetaldehyde 123-35-3, Myrcene  
123-42-2, 4-Hydroxy-4-methyl-2-pentanone 123-51-3, Iso-Amyl alcohol  
123-72-8, Butanal 124-07-2, Octanoic acid, biological studies  
124-13-0, Octanal 124-19-6, Nonanal 126-33-0, Tetrahydrothiophene,  
1,1,dioxide 127-91-3,  $\beta$ -Pinene 128-37-0, Ionol, biological  
studies 137-32-6, 2-Methylbutan-1-ol 138-86-3, Limonene 142-62-1,  
Caproic acid, biological studies 142-91-6, Isopropyl palmitate  
149-57-5, 2-Ethylhexanoic acid 289-16-7, 1,2,4-Trithiolane 291-22-5,  
1,2,4,5-Tetrathiane 292-45-5, 1,2,4,6-Tetrathiepane 470-82-6,  
1,8-Cineole 473-13-2,  $\alpha$ -Selinene 483-76-1,  $\delta$ -Cadinene  
483-78-3, Cadalene 502-61-4, Farnesene 506-42-3,  
trans-9-Octadecen-1-ol 512-61-8, Santalene 513-86-0, Acetoin  
514-51-2,  $\beta$ -Patchoulene 536-74-3, Phenylacetylene 541-85-5,  
5-Methyl-3-heptanone 555-10-2,  $\beta$ -Phellandrene 579-07-7,  
1-Phenyl-1,2-propanedione 582-24-1,  
 $\alpha$ -Hydroxyacetophenone 586-62-9, Terpinolene 589-82-2, 3-Heptanol  
589-98-0, Octan-3-ol 616-25-1, Pent-1-en-3-ol 617-94-7,



$\alpha,\alpha$ -Dimethylbenzenemethanol 623-36-9 624-92-0, Dimethyl  
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 928-96-1, cis-Hex-3-en-1-ol 930-60-9, 2-Cyclopentene-1,4-dione  
 933-48-2, Trixanol 1454-85-9, 1-Heptadecanol 1576-95-0, cis-2-Pentenol  
 1618-26-4, 2,4-Dithiapentane 1620-98-0,  
 3,5-Di-tert-butyl-4-hydroxybenzaldehyde 1741-83-9, 2-Thiaheptane  
 1795-15-9, Octylcyclohexane 1879-07-8, cis-p-Menth-8-ene 1879-09-0,  
 6-tert-Butyl-2,4-dimethyl phenol 2277-20-5, 6-Nonenal, (E)- 2314-48-9,  
 Carbonotrithioic acid dimethyl ester 2436-90-0, Citronellene  
 3338-55-4, cis- $\beta$ -Ocimene 3387-41-5, Sabinene 3391-86-4,  
 1-Octen-3-ol 3491-57-4 3592-19-6 3658-80-8, Dimethyl trisulfide  
 3777-69-3, 2-Pentylfuran 3913-02-8, 2-Butyl octanol 4130-42-1,  
 2,6-Bis(1,1-dimethylethyl)-4-ethylphenol 4170-30-3, 2-Butenal  
 4312-99-6, 1-Octen-3-one 4630-07-3, Valencene 4829-04-3,  
 1,3-Dithiolane 5008-72-0 5418-86-0 6540-86-9, 2,4,6-Trithiaheptane  
 6617-49-8 6728-26-3, trans-Hex-2-en-1-al 6753-98-6, Humulene  
 6938-51-8, 2-Octylbenzoate 10522-26-6, 2-Methyl-1-undecanol 13877-93-5  
 15193-25-6, o-Menth-8-ene 16225-26-6, 3,5-Di-tert-butylbenzoic acid  
 16630-52-7, 3-Methylthiobutanal 17066-67-0,  $\beta$ -Selinene  
 17283-81-7, Dihydro  $\beta$ -ionone 17699-14-8,  $\alpha$ -Cubebene  
 18794-84-8, Trans- $\beta$ -Farnesene 19780-25-7, 2-Ethyl-2-butenal  
 20068-02-4 23986-74-5, Germacrene D 27070-58-2, Octadecene  
 27251-68-9, Pentadecene 27625-35-0, 3-Methylbutyl 2-methylbutyrate  
 33577-16-1 38514-13-5, 3-Ethyl-4-methyl-1-pentanol 38634-59-2,  
 Methylthiomethyl acetyl sulfide 42474-44-2, 2,3,5-Trithiahexane  
 51154-96-2, Massoialactone 58809-73-7, 2-Methylthiopropionic acid  
 66537-39-1 66537-40-4 80466-34-8, 2,4-Hexadienal 85544-38-3,  
 2,4,5,7-Tetrathiaoctane 103240-92-2 117210-66-9 119117-00-9  
 415686-96-3 415687-00-2  
 RL: ANT (Analyte); BSU (Biological study, unclassified); OCU (Occurrence,  
 unclassified); ANST (Analytical study); BIOL (Biological study); OCCU  
 (Occurrence)  
 (headspace aroma of wild onion trees)

L29 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2000:871753 HCAPLUS

DOCUMENT NUMBER: 134:99830

TITLE: m-Dimethoxybenzene

AUTHOR(S): Letizia, C. S.; Cocchiara, J.; Wellington, G. A.;

Funk, C.; Api, A. M.

CORPORATE SOURCE: Research Institute for Fragrance Materials, Inc.,  
 Hackensack, NJ, 07601, USA

SOURCE: Food and Chemical Toxicology (2000), 38(Suppl. 3),  
 S59-S62

PUBLISHER: CODEN: FCTOD7; ISSN: 0278-6915

DOCUMENT TYPE: Elsevier Science Ltd.

LANGUAGE: Journal

ABSTRACT: English

M-Dimethoxybenzene is approved by FDA for food use and was given Generally  
 Recognized As Safe status as a flavor ingredient by Flavor and Extract  
 Manufacturers' Association The Council of Europe (1992) included  
 m-dimethoxybenzene in Category A flavoring substances, which may be used in  
 foodstuffs.

SO Food and Chemical Toxicology (2000), 38(Suppl. 3), S59-S62

CODEN: FCTOD7; ISSN: 0278-6915

AB M-Dimethoxybenzene is approved by FDA for food use and was given Generally  
 Recognized As Safe status as a flavor ingredient by Flavor and Extract  
 Manufacturers' Association The Council of Europe (1992) included

m-dimethoxybenzene in Category A flavoring substances, which may be used in foodstuffs.

ST dimethoxybenzene flavoring food

IT Flavoring materials  
(dimethoxybenzene as flavoring agent for food use)

IT 151-10-0  
RL: BUU (Biological use, unclassified); FFD (Food or feed use); BIOL (Biological study); USES (Uses)  
(dimethoxybenzene as flavoring agent for food use)

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

SO Food and Chemical Toxicology (2000), 38(Suppl. 3), S59-S62  
CODEN: FCTOD7; ISSN: 0278-6915

AB M-Dimethoxybenzene is approved by FDA for food use and was given Generally Recognized As Safe status as a flavor ingredient by Flavor and Extract Manufacturers' Association The Council of Europe (1992) included m-dimethoxybenzene in Category A flavoring substances, which may be used in foodstuffs.

ST dimethoxybenzene flavoring food

IT Flavoring materials  
(dimethoxybenzene as flavoring agent for food use)

IT 151-10-0  
RL: BUU (Biological use, unclassified); FFD (Food or feed use); BIOL (Biological study); USES (Uses)  
(dimethoxybenzene as flavoring agent for food use)

L29 ANSWER 5 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2000:128824 HCAPLUS

DOCUMENT NUMBER: 132:149046

TITLE: The flavor composition of umbelliferous fruits. Part 1. Anise (Pimpinella anisum)

AUTHOR(S): Kollmannsberger, H.; Fricke, G.; Paulus, H.; Nitz, S.  
CORPORATE SOURCE: Institut für Lebensmitteltechnologie und Analytische Chemie, Technische Universität München, Freising, D-85350, Germany

SOURCE: Advances in Food Sciences (2000), 22(1/2), 47-61  
CODEN: AFSCF2; ISSN: 1431-7737

PUBLISHER: Advances in Food Sciences

DOCUMENT TYPE: Journal

LANGUAGE: German

ABSTRACT:

Aniseed (P. anisum) was extracted with diethylether (LSM), simultaneous distillation extraction (SDE) and CO<sub>2</sub> supercrit. fluid extraction (SFE). The flavor composition of the

exts. was investigated by gaschromatog. - mass spectrometry (GC-MS) with simultaneous effluent sniffing detection. 150 Substances (e.g. 22 monoterpenoids, 32 sesquiterpenoids, 52 phenolic or aromatic compds.) and 20 not aromatic esters could be identified. The occurrence of isomeric pseudo-isoeugenols and pseudo-isoeugenol methylethers, pseudo-isovanillyl-2-methylbutanoate, some O-containing and aromatic himachalene derivs., as well as isomeric himachalatriens could be confirmed. The most odoriferous flavor compds. were trans-anethol and ethyl-2-methylbutanoate in all exts. SFE and LSM exts. show a remarkable higher content in higher boiling components (e.g. vanillin with its strong sweet flavor). The amount of low boiling compds. is very similar in all exts. Nevertheless some odoriferous trace components like methional, phenylacetaldehyde and other thermal induced artifacts impart a typical cooking flavor note to the distillate. These differences are regarded to be responsible for the bad sensorial quality of the distillate compared to the other exts.

TI The flavor composition of umbelliferous fruits. Part 1. Anise

(*Pimpinella anisum*)

SO Advances in Food Sciences (2000), 22(1/2), 47-61  
CODEN: AFSCFP; ISSN: 1431-7737

AB Aniseed (*P. anisum*) was extracted with diethylether (LSM), simultaneous distillation extraction (SDE) and CO<sub>2</sub> supercrit. fluid extraction (SFE). The flavor composition of the exts. was investigated by gaschromatog. - mass spectrometry (GC-MS) with simultaneous effluent sniffing detection. 150 Substances (e.g. . . pseudo-isoeugenol methylethers, pseudo-isovanillyl-2-methylbutanoate, some O-containing and aromatic himachalene derivs., as well as isomeric himachalatriens could be confirmed. The most odoriferous flavor compds. were trans-anethol and ethyl-2-methylbutanoate in all exts. SFE and LSM exts. show a remarkable higher content in higher boiling components (e.g. vanillin with its strong sweet flavor). The amount of low boiling compds. is very similar in all exts. Nevertheless some odoriferous trace components like methional, phenylacetaldehyde and other thermal induced artifacts impart a typical cooking flavor note to the distillate. These differences are regarded to be responsible for the bad sensorial quality of the distillate compared. . .

ST Anise seed flavor essential oil volatile GCMS; *Pimpinella* seed flavor essential oil volatile GCMS

IT Anise  
Flavor  
Volatile substances  
(flavor composition of *Pimpinella anisum* determined by GC/MS)

IT Essential oils  
Monoterpenes  
Sesquiterpenes  
RL: ANT (Analyte); BOC (Biological occurrence); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence)  
(flavor composition of *Pimpinella anisum* determined by GC/MS)

IT 60-12-8, Phenyl ethanol 66-25-1, Hexanal 76-22-2, Camphor 78-70-6, Linalool 79-77-6,  $\beta$ -Ionone 79-92-5, Camphene 80-56-8,  $\alpha$ -Pinene 89-80-5, Menthone 90-02-8, 2-Hydroxy-benzaldehyde, biological studies 90-05-1, Guaiacol 93-02-7, 2,5-Dimethoxy-benzaldehyde 94-30-4, Ethyl anisate 98-01-1, Furfural, biological studies 98-55-5,  $\alpha$ -Terpineol 99-49-0, Carvone 99-85-4,  $\gamma$ -Terpinene 99-87-6, p-Cymene 100-06-1 100-09-4, p-Methoxy benzoic acid 100-42-5, Styrol, biological studies 100-51-6, Benzyl alcohol, biological studies 100-52-7, Benzaldehyde, biological studies 100-66-3, Anisol, biological studies 104-45-0 104-46-1D, Anethol, dimers 105-13-5, Anisic alcohol 111-27-3, Hexanol, biological studies 111-61-5, Ethyl octadecanoate 112-39-0, Methyl hexadecanoate 112-61-8, Methyl octadecanoate 116-53-0, 2-Methyl butyric acid 121-33-5, Vanillin 121-97-1 121-98-2 122-00-9, p-Methylacetophenone 122-78-1, Phenylacetaldehyde 122-84-9 123-11-5, Anis aldehyde, biological studies 123-11-5D, Anisaldehyde, dimer, biological studies 123-35-3, Myrcene 124-06-1, Ethyl tetradecanoate 124-10-7, Methyl tetradecanoate 124-13-0, Octanal 127-91-3,  $\beta$ -Pinene 138-86-3, Limonene 140-67-0, Methylchavicol 142-62-1, Hexanoic acid, biological studies 150-76-5, p-Methoxyphenol 150-86-7, Phytol 301-00-8 470-82-6, 1,8-Cineol 483-76-1,  $\delta$ -Cadinene 483-77-2, Calamenene 483-78-3, Cadalone 491-07-6, Iso-menthone 495-60-3,  $\alpha$ -Zingiberene 495-61-4,  $\beta$ -Bisabolene 502-69-2 503-74-2, 3-Methyl butyric acid 504-96-1, Neophytadiene 507-70-0, Borneol 515-13-9,  $\beta$ -Elemene 546-80-5, Thujone 562-74-3 584-82-7 585-25-1, 2,3-Octanedione 628-97-7, Ethyl hexadecanoate 644-30-4 673-22-3 868-57-5, Methyl-2-methylbutanoate 928-68-7 1003-29-8, 2-Formyl pyrrole 1072-83-9, 2-Acetyl pyrrole 1137-12-8,

Longicyclene 1195-79-5, Fenchone 1461-03-6,  $\beta$ -Himachalene  
 2436-90-0,  $\beta$ -Citronellene 2445-67-2, Isobutyl-2-methylbutanoate  
 2445-78-5, 2-Methylbutyl-2-methylbutanoate 2777-58-4 3268-49-3,  
 Methional 3319-15-1 3380-68-5 3387-41-5, Sabinene 3853-83-6,  
 $\alpha$ -Himachalene 3856-25-5,  $\alpha$ -Copaene 4180-23-8,  
 trans-Anethol 4312-99-6, 1-Octen-3-one 5025-38-7 5349-60-0  
 5975-49-5, Isogerjere 5989-08-2,  $\alpha$ -Longipinene 6728-26-3  
 6750-60-3, Spathulenol 6902-73-4D, Geijerene, derivs. 7132-64-1,  
 Methyl pentadecanoate 7370-44-7, 5-Hexadecanolide 7452-79-1,  
 Ethyl-2-methylbutanoate 7784-99-8, Vinylguaiacol 10032-15-2,  
 Hexyl-2-methylbutanoate 13391-27-0 13474-59-4 14912-44-8,  
 $\alpha$ -Ylangene 17627-44-0,  $\alpha$ -Bisabolene 18794-84-8  
 18829-56-6 19419-67-1, ar-Himachalene 19754-22-4 19785-01-4  
 19785-02-5 20307-83-9,  $\beta$ -Sesquiphellandrene 20307-84-0,  
 $\delta$ -Elemene 21391-99-1,  $\alpha$ -Calacorene 23726-93-4,  
 $\beta$ -Damascenone 25679-28-1 27625-35-0,  
 3-Methylbutyl-2-methylbutanoate 27739-28-2 28061-47-4 29960-49-4  
 30314-64-8 34302-52-8 41587-31-9, Vinylnisole 50277-34-4,  
 $\beta$ -Calacorene 51766-65-5 53111-25-4,  $\gamma$ -Himachalene  
 56144-27-5 58989-20-1 60026-20-2 60784-31-8 64825-84-9  
 64825-85-0 71672-25-8, Ethyl octadecadienoate 78204-62-3 78446-77-2  
 88395-46-4, Iso-spathulenol 97180-28-4 98755-19-2 98755-22-7  
 106871-14-1 115569-82-9 121198-16-1, Ethyl octadecatrienoate  
 150133-25-8 227960-21-6, Himachal-2-en-6-ol 257887-98-2 257888-07-6  
 257888-10-1 257888-13-4 257888-15-6

RL: ANT (Analyte); BOC (Biological occurrence); BSU (Biological study,  
 unclassified); ANST (Analytical study); BIOL (Biological study); OCCU  
 (Occurrence)

(flavor composition of *Pimpinella anisum* determined by GC/MS)

OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD  
 (7 CITINGS)

REFERENCE COUNT: 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

TI The flavor composition of umbelliferous fruits. Part 1. Anise  
 (*Pimpinella anisum*)

SO Advances in Food Sciences (2000), 22(1/2), 47-61  
 CODEN: AFSCF2; ISSN: 1431-7737

AB Aniseed (*P. anisum*) was extracted with diethylether (LSM), simultaneous  
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extraction (SDE) and CO<sub>2</sub> supercrit. fluid extraction (SFE). The flavor  
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the exts. was investigated by gaschromatog. - mass spectrometry (GC-MS)  
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 pseudo-isoeugenols and pseudo-isoeugenol methylethers,  
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derivs., as well as isomeric himachalatriens could be confirmed. The most  
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 phenylacetaldehyde and other thermal induced artifacts impart a typical  
 cooking flavor note to the distillate. These differences are regarded  
 to be responsible for the bad sensorial quality of the distillate compared  
 to the other exts.

ST Anise seed flavor essential oil volatile GCMS; *Pimpinella* seed flavor  
 essential oil volatile GCMS

IT Anise

Flavor

Volatile substances

(flavor composition of *Pimpinella anisum* determined by GC/MS)

IT Essential oils

Monoterpenes

Sesquiterpenes

RL: ANT (Analyte); BOC (Biological occurrence); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence)

(flavor composition of *Pimpinella anisum* determined by GC/MS)

- IT 60-12-8, Phenyl ethanol 66-25-1, Hexanal 76-22-2, Camphor 78-70-6, Linalool 79-77-6,  $\beta$ -Ionone 79-92-5, Camphene 80-56-8,  $\alpha$ -Pinene 89-80-5, Menthone 90-02-8, 2-Hydroxy-benzaldehyde, biological studies 90-05-1, Guaiacol 93-02-7, 2,5-Dimethoxy-benzaldehyde 94-30-4, Ethyl anisate 98-01-1, Furfural, biological studies 98-55-5,  $\alpha$ -Terpineol 99-49-0, Carvone 99-85-4,  $\gamma$ -Terpinene 99-87-6, p-Cymene 100-06-1 100-09-4, p-Methoxy benzoic acid 100-42-5, Styrol, biological studies 100-51-6, Benzyl alcohol, biological studies 100-52-7, Benzaldehyde, biological studies 100-66-3, Anisol, biological studies 104-45-0 104-46-1D, Anethol, dimers 105-13-5, Anisic alcohol 111-27-3, Hexanol, biological studies 111-61-5, Ethyl octadecanoate 112-39-0, Methyl hexadecanoate 112-61-8, Methyl octadecanoate 116-53-0, 2-Methyl butyric acid 121-33-5, Vanillin 121-97-1 121-98-2 122-00-9, p-Methylacetophenone 122-78-1, Phenylacetaldehyde 122-84-9 123-11-5, Anis aldehyde, biological studies 123-11-5D, Anisaldehyde, dimer, biological studies 123-35-3, Myrcene 124-06-1, Ethyl tetradecanoate 124-10-7, Methyl tetradecanoate 124-13-0, Octanal 127-91-3,  $\beta$ -Pinene 138-86-3, Limonene 140-67-0, Methylchavicol 142-62-1, Hexanoic acid, biological studies 150-76-5, p-Methoxyphenol 150-86-7, Phytol 301-00-8 470-82-6, 1,8-Cineol 483-76-1,  $\delta$ -Cadinene 483-77-2, Calamene 483-78-3, Cadalene 491-07-6, Iso-menthone 495-60-3,  $\alpha$ -Zingiberene 495-61-4,  $\beta$ -Bisabolene 502-69-2 503-74-2, 3-Methyl butyric acid 504-96-1, Neophytadiene 507-70-0, Borneol 515-13-9,  $\beta$ -Elemene 546-80-5, Thujone 562-74-3 584-82-7 585-25-1, 2,3-Octanedione 628-97-7, Ethyl hexadecanoate 644-30-4 673-22-3 868-57-5, Methyl-2-methylbutanoate 928-68-7 1003-29-8, 2-Formyl pyrrole 1072-83-9, 2-Acetyl pyrrole 1137-12-8, Longicyclene 1195-79-5, Fenchone 1461-03-6,  $\beta$ -Himachalene 2436-90-0,  $\beta$ -Citronellene 2445-67-2, Isobutyl-2-methylbutanoate 2445-78-5, 2-Methylbutyl-2-methylbutanoate 2777-58-4 3268-49-3, Methional 3319-15-1 3380-68-5 3387-41-5, Sabinene 3853-83-6,  $\alpha$ -Himachalene 3856-25-5,  $\alpha$ -Copaene 4180-23-8, trans-Anethol 4312-99-6, 1-Octen-3-one 5025-38-7 5349-60-0 5975-49-5, Isogeijerene 5989-08-2,  $\alpha$ -Longipinene 6728-26-3 6750-60-3, Spathulenol 6902-73-4D, Geijerene, derivs. 7132-64-1, Methyl pentadecanoate 7370-44-7, 5-Hexadecanolide 7452-79-1, Ethyl-2-methylbutanoate 7784-99-8, Vinylguaiacol 10032-15-2, Hexyl-2-methylbutanoate 13391-27-0 13474-59-4 14912-44-8,  $\alpha$ -Ylangene 17627-44-0,  $\alpha$ -Bisabolene 18794-84-8 18829-56-6 19419-67-1, ar-Himachalene 19754-22-4 19785-01-4 19785-02-5 20307-83-9,  $\beta$ -Sesquiphellandrene 20307-84-0,  $\delta$ -Elemene 21391-99-1,  $\alpha$ -Calacorene 23726-93-4,  $\beta$ -Damascenone 25679-28-1 27625-35-0, 3-Methylbutyl-2-methylbutanoate 27739-28-2 28061-47-4 29960-49-4 30314-64-8 34302-52-8 41587-31-9, Vinylanisole 50277-34-4,  $\beta$ -Calacorene 51766-65-5 53111-25-4,  $\gamma$ -Himachalene 56144-27-5 58989-20-1 60026-20-2 60784-31-8 64825-84-9 64825-85-0 71672-25-8, Ethyl octadecadienoate 78204-62-3 78446-77-2 88395-46-4, Iso-spathulenol 97180-28-4 98755-19-2 98755-22-7 106871-14-1 115569-82-9 121198-16-1, Ethyl octadecatrienoate

150133-25-8 227960-21-6, Himachal-2-en-6-ol 257887-98-2 257888-07-6  
257888-10-1 257888-13-4 257888-15-6  
RL: ANT (Analyte); BOC (Biological occurrence); BSU (Biological study,  
unclassified); ANST (Analytical study); BIOL (Biological study); OCCU  
(Occurrence)  
(flavor composition of Pimpinella anisum determined by GC/MS)

L29 ANSWER 6 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1998:256643 HCAPLUS

DOCUMENT NUMBER: 128:243078

ORIGINAL REFERENCE NO.: 128:48133a, 48136a

TITLE: New Components with Potential Antioxidant and  
Organoleptic Properties, Detected for the First Time  
in Liquid Smoke Flavoring Preparations

AUTHOR(S): Guillen, Maria D.; Ibargoitia, Maria L.

CORPORATE SOURCE: Tecnologia de Alimentos Facultad de Farmacia,  
Universidad del Pais Vasco, Vitoria, 01006, Spain  
SOURCE: Journal of Agricultural and Food Chemistry (1998),  
46(4), 1276-1285

CODEN: JAFCAU; ISSN: 0021-8561

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

ABSTRACT:

A com. aqueous smoke preparation was exhaustively extracted, using dichloromethane as solvent, until the carrier had totally lost its smoky odor. Qual. and quant. characterizations of the extract were performed by means of gas chromatog./mass spectrometry and gas chromatog. with flame ionization detector, resp. Carbonyl derivs. including aldehydes and ketones as well as acids and esters are almost absent; however, the high proportion of phenol, guaiacol, and syringol derivs. is noticeable. The presence of di-tert-butylhydroxytoluene, several hopanes, and a number of lignin dimers must be pointed out; these latter components had apparently not been detected before either in smoke flavorings or in wood smoke. The mass spectral data of the compds. considered as lignin dimers and of the unidentified components are given. The presence of lignin dimers is very interesting from the point of view of health and food technol. for their therapeutic, organoleptic, and antioxidant properties.

TI New Components with Potential Antioxidant and Organoleptic Properties,  
Detected for the First Time in Liquid Smoke Flavoring Preparations

SO Journal of Agricultural and Food Chemistry (1998), 46(4), 1276-1285  
CODEN: JAFCAU; ISSN: 0021-8561

AB . . . number of lignin dimers must be pointed out; these latter components  
had apparently not been detected before either in smoke flavorings or in  
wood smoke. The mass spectral data of the compds. considered as lignin  
dimers and of the unidentified components. . .

ST smoke flavoring compn

IT Alcohols, biological studies

Aldehydes, biological studies

Aromatic hydrocarbons, biological studies

Ethers, biological studies

Ketones, biological studies

Phenols, biological studies

Terpenes, biological studies

RL: BAC (Biological activity or effector, except adverse); BOC (Biological  
occurrence); BSU (Biological study, unclassified); BIOL (Biological  
study); OCCU (Occurrence)

(components with potential antioxidant and organoleptic properties,  
detected for the first time in liquid smoke flavoring)

IT Triterpenes

RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)

(hopane; components with potential antioxidant and organoleptic properties, detected for the first time in liquid smoke flavoring)

IT Flavoring materials

(smoke flavors; components with potential antioxidant and organoleptic properties, detected for the first time in liquid smoke flavoring)

- IT 60-12-8, 2-Phenylethanol 64-19-7, Acetic acid, biological studies  
67-64-1, 2-Propanone, biological studies 75-07-0, Acetaldehyde, biological studies 78-93-3, 2-Butanone, biological studies 85-01-8, Phenanthrene, biological studies 88-18-6, 2-(1,1-Dimethylethyl)phenol 89-83-8, Thymol 90-00-6, 2-Ethylphenol 90-05-1, Guaiacol 91-10-1, Syringol 91-16-7 91-20-3, Naphthalene, biological studies 93-15-2 93-16-3 93-51-6, 4-Methylguaiacol 95-48-7, 2-Methylphenol, biological studies 95-87-4, 2,5-Dimethylphenol 97-53-0, Eugenol 98-00-0, Furfuryl alcohol 98-86-2, Acetophenone, biological studies 99-49-0, Carvone 99-87-6, p-Cymene 100-42-5, biological studies 100-51-6, Benzyl alcohol, biological studies 100-52-7, Benzaldehyde, biological studies 102-25-0, 1,3,5-Triethylbenzene 104-87-0, 4-Methylbenzaldehyde 105-67-9, 2,4-Dimethylphenol 106-44-5, biological studies 108-39-4, biological studies 108-68-9, 3,5-Dimethylphenol 108-95-2, Phenol, biological studies 111-02-4, Squalene 112-95-8, Eicosane 121-33-5, Vanillin 121-34-6, Vanillic acid 134-96-3, Syringaldehyde 140-67-0, Estragole 150-78-7, 1,4-Dimethoxybenzene 151-10-0, 1,3-Dimethoxybenzene 458-35-5, Coniferyl alcohol 470-82-6, Eucalyptol 487-11-6, 5-(2-Propenyl)-1,2,3-trimethoxybenzene 487-12-7 494-99-5, 3,4-Dimethoxytoluene 496-78-6, 2,4,5-Trimethylphenol 498-02-2, Acetovanillone 499-75-2, Carvacrol 526-75-0, 2,3-Dimethylphenol 526-85-2, 2,3,4-Trimethylphenol 527-60-6, 2,4,6-Trimethylphenol 539-12-8, 4-Propenylphenol 544-76-3, Hexadecane 544-85-4, Dotriacontane 576-26-1 577-16-2, 1-(2-Methylphenyl)ethanone 585-34-2, 3-(1,1-Dimethylethyl)phenol 593-45-3, Octadecane 593-49-7, Heptacosane 620-17-7, 3-Ethylphenol 629-59-4, Tetracosane 629-78-7, Heptadecane 629-92-5, Nonadecane 629-94-7, Heneicosane 629-97-0, Docosane 629-99-2, Pentacosane 630-01-3, Hexacosane 630-02-4, Octacosane 630-03-5, Nonacosane 630-04-6, Hentriacontane 630-05-7, Tritriacontane 634-36-6, 1,2,3-Trimethoxybenzene 638-67-5, Tricosane 638-68-6, Triacotane 644-35-9, 2-Propylphenol 645-56-7, 4-Propylphenol 646-31-1, Tetracosane 697-82-5, 2,3,5-Trimethylphenol 698-71-5, 3-Ethyl-5-methylphenol 705-15-7 719-22-2, 2,6-Bis(1,1-dimethylethyl)-2,5-cyclohexadiene-1,4-dione 832-69-9, 1-Methylphenanthrene 944-99-0, 2,6-Dimethoxyphenyl acetate 1121-05-7 1123-94-0, 4-Ethyl-3-methylphenol 1136-86-3 1192-62-7 1620-98-0, 4-Hydroxy-3,5-di-tert-butylbenzaldehyde 1655-68-1 2033-89-8, 3,4-Dimethoxyphenol 2416-94-6 2478-38-8, 1-(4-Hydroxy-3,5-dimethoxyphenyl)ethanone 2503-46-0 2758-18-1 2785-87-7, 4-Propylguaiacol 2785-89-9, 4-Ethylguaiacol 3194-15-8 3840-31-1 5779-72-6, 2,4,5-Trimethylbenzaldehyde 5912-86-7, cis-Isoeugenol 5932-68-3, trans-Isoeugenol 6004-60-0 6627-88-9 6635-22-9 6638-05-7, 4-Methylsyringol 6766-82-1, 4-Propylsyringol 7786-61-0, 4-Vinylguaiacol 13849-96-2, 17 $\alpha$ (H), 21 $\beta$ (H)-Hopane 14059-92-8, 4-Ethylsyringol 14167-59-0, Tetraatriacontane 18435-45-5, 1-Nonadecene 18435-54-6, 1-Hentriacontene 20983-15-7 24810-59-1 26998-80-1, Trimethylphenol 27587-17-3, 2-Methyl-1,4-benzenedicarboxaldehyde 28343-22-8, 4-Vinylsyringol 28777-87-9, Hydroxybenzaldehyde 28790-86-5, 2,3,4-Trimethyl-2-cyclopenten-1-one 30434-65-2 32556-65-3 39831-51-1 53584-62-6, Homohopane 53951-50-1, Ethylbenzaldehyde 54311-28-3,

Bishomohopane 55683-21-1, 3,4,5-Trimethyl-2-cyclopenten-1-one  
59893-87-7 60553-44-8 61868-12-0, 1-Tetratriacontene 66309-82-8  
69271-91-6 71629-80-6, Trishomohopane 71880-75-6 79755-53-6  
81825-21-0 82000-05-3 120550-70-1 204781-71-5 204781-72-6,  
A'-Neo-28-norgammacerane 204781-73-7 204781-74-8

RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)

(components with potential antioxidant and organoleptic properties, detected for the first time in liquid smoke flavoring)

OS.CITING REF COUNT: 50 THERE ARE 50 CAPLUS RECORDS THAT CITE THIS RECORD (51 CITINGS)

REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

TI New Components with Potential Antioxidant and Organoleptic Properties, Detected for the First Time in Liquid Smoke Flavoring Preparations

SO Journal of Agricultural and Food Chemistry (1998), 46(4), 1276-1285  
CODEN: JAFCAU; ISSN: 0021-8561

AB A com. aqueous smoke preparation was exhaustively extracted, using dichloromethane as

solvent, until the carrier had totally lost its smoky odor. Qual. and quant. characterizations of the extract were performed by means of gas chromatog./mass spectrometry and gas chromatog. with flame ionization detector, resp. Carbonyl derivs. including aldehydes and ketones as well as acids and esters are almost absent; however, the high proportion of phenol, guaiacol, and syringol derivs. is noticeable. The presence of di-tert-butylhydroxytoluene, several hopanes, and a number of lignin dimers must be pointed out; these latter components had apparently not been detected before either in smoke flavorings or in wood smoke. The mass spectral data of the compds. considered as lignin dimers and of the unidentified components are given. The presence of lignin dimers is very interesting from the point of view of health and food technol. for their therapeutic, organoleptic, and antioxidant properties.

ST smoke flavoring compn

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Aldehydes, biological studies  
Aromatic hydrocarbons, biological studies  
Ethers, biological studies  
Ketones, biological studies  
Phenols, biological studies  
Terpenes, biological studies

RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)

(components with potential antioxidant and organoleptic properties, detected for the first time in liquid smoke flavoring)

IT Triterpenes

RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)

(hopane; components with potential antioxidant and organoleptic properties, detected for the first time in liquid smoke flavoring)

IT Flavoring materials

(smoke flavors; components with potential antioxidant and organoleptic properties, detected for the first time in liquid smoke flavoring)

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67-64-1, 2-Propanone, biological studies 75-07-0, Acetaldehyde, biological studies 78-93-3, 2-Butanone, biological studies 85-01-8, Phenanthrene, biological studies 88-18-6, 2-(1,1-Dimethylethyl)phenol



89-83-8, Thymol 90-00-6, 2-Ethylphenol 90-05-1, Guaiacol 91-10-1, Syringol 91-16-7 91-20-3, Naphthalene, biological studies 93-15-2 93-16-3 93-51-6, 4-Methylguaiacol 95-48-7, 2-Methylphenol, biological studies 95-87-4, 2,5-Dimethylphenol 97-53-0, Eugenol 98-00-0, Furfuryl alcohol 98-86-2, Acetophenone, biological studies 99-49-0, Carvone 99-87-6, p-Cymene 100-42-5, biological studies 100-51-6, Benzyl alcohol, biological studies 100-52-7, Benzaldehyde, biological studies 102-25-0, 1,3,5-Triethylbenzene 104-87-0, 4-Methylbenzaldehyde 105-67-9, 2,4-Dimethylphenol 106-44-5, biological studies 108-39-4, biological studies 108-68-9, 3,5-Dimethylphenol 108-95-2, Phenol, biological studies 111-02-4, Squalene 112-95-8, Eicosane 121-33-5, Vanillin 121-34-6, Vanillic acid 134-96-3, Syringaldehyde 140-67-0, Estragole 150-78-7, 1,4-Dimethoxybenzene 151-10-0, 1,3-Dimethoxybenzene 458-35-5, Coniferyl alcohol 470-82-6, Eucalyptol 487-11-6, 5-(2-Propenyl)-1,2,3-trimethoxybenzene 487-12-7 494-99-5, 3,4-Dimethoxytoluene 496-78-6, 2,4,5-Trimethylphenol 498-02-2, Acetovanillone 499-75-2, Carvacrol 526-75-0, 2,3-Dimethylphenol 526-85-2, 2,3,4-Trimethylphenol 527-60-6, 2,4,6-Trimethylphenol 539-12-8, 4-Propenylphenol 544-76-3, Hexadecane 544-85-4, Dotriacontane 576-26-1 577-16-2, 1-(2-Methylphenyl)ethanone 585-34-2, 3-(1,1-Dimethylethyl)phenol 593-45-3, Octadecane 593-49-7, Heptacosane 620-17-7, 3-Ethylphenol 629-59-4, Tetradecane 629-78-7, Heptadecane 629-92-5, Nonadecane 629-94-7, Heneicosane 629-97-0, Docosane 629-99-2, Pentacosane 630-01-3, Hexacosane 630-02-4, Octacosane 630-03-5, Nonacosane 630-04-6, Hentriacontane 630-05-7, Tritriacontane 634-36-6, 1,2,3-Trimethoxybenzene 638-67-5, Tricosane 638-68-6, Triacotane 644-35-9, 2-Propylphenol 645-56-7, 4-Propylphenol 646-31-1, Tetracosane 697-82-5, 2,3,5-Trimethylphenol 698-71-5, 3-Ethyl-5-methylphenol 705-15-7 719-22-2, 2,6-Bis(1,1-dimethylethyl)-2,5-cyclohexadiene-1,4-dione 832-69-9, 1-Methylphenanthrene 944-99-0, 2,6-Dimethoxyphenyl acetate 1121-05-7 1123-94-0, 4-Ethyl-3-methylphenol 1136-86-3 1192-62-7 1620-98-0, 4-Hydroxy-3,5-di-tert-butylbenzaldehyde 1655-68-1 2033-89-8, 3,4-Dimethoxyphenol 2416-94-6 2478-38-8, 1-(4-Hydroxy-3,5-dimethoxyphenyl)ethanone 2503-46-0 2758-18-1 2785-87-7, 4-Propylguaiacol 2785-89-9, 4-Ethylguaiacol 3194-15-8 3840-31-1 5779-72-6, 2,4,5-Trimethylbenzaldehyde 5912-86-7, cis-Isoeugenol 5932-68-3, trans-Isoeugenol 6004-60-0 6627-88-9 6635-22-9 6638-05-7, 4-Methylsyringol 6766-82-1, 4-Propylsyringol 7786-61-0, 4-Vinylguaiacol 13849-96-2, 17 $\alpha$ (H),21 $\beta$ (H)-Hopane 14059-92-8, 4-Ethylsyringol 14167-59-0, Tetratriacontane 18435-45-5, 1-Nonadecene 18435-54-6, 1-Hentriacontene 20983-15-7 24810-59-1 26998-80-1, Trimethylphenol 27587-17-3, 2-Methyl-1,4-benzenedicarboxaldehyde 28343-22-8, 4-Vinylsyringol 28777-87-9, Hydroxybenzaldehyde 28790-86-5, 2,3,4-Trimethyl-2-cyclopenten-1-one 30434-65-2 32556-65-3 39831-51-1 53584-62-6, Homohopane 53951-50-1, Ethylbenzaldehyde 54311-28-3, Bishomohopane 55683-21-1, 3,4,5-Trimethyl-2-cyclopenten-1-one 59893-87-7 60553-44-8 61868-12-0, 1-Tetratriacontene 66309-82-8 69271-91-6 71629-80-6, Trishomohopane 71880-75-6 79755-53-6 81825-21-0 82000-05-3 120550-70-1 204781-71-5 204781-72-6, A'-Neo-28-norgammacerane 204781-73-7 204781-74-8

RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)

(components with potential antioxidant and organoleptic properties, detected for the first time in liquid smoke flavoring)

DOCUMENT NUMBER: 126:108688  
 Correction of: 125:95620  
 ORIGINAL REFERENCE NO.: 126:20923a  
 TITLE: Antiplaque, antigingivitis oral compositions  
 containing phosphates and copper sources  
 INVENTOR(S): Sanker, Lowell Alan; Upson, James Grigg  
 PATENT ASSIGNEE(S): Procter and Gamble Company, USA  
 SOURCE: PCT Int. Appl., 17 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9615768	A1	19960530	WO 1995-US14013	19951027 <--
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, UZ, VN				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9540160	A	19960617	AU 1995-40160	19951027 <--
IN 1995DE02032	A	20050311	IN 1995-DE2032	19951106
US 5628986	A	19970513	US 1996-632936	19960416 <--
PRIORITY APPLN. INFO.:			US 1994-341716	A 19941118
			WO 1995-US14013	W 19951027

# ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

## ABSTRACT:

Disclosed are oral compns. such as toothpastes, mouth rinses, lozenges, and gums containing at least one phosphate derivative and a copper source. A mouthwash contained water 70.86, sorbitol solution (70 %) 10.25, Na saccharin 0.08, ethanol 10.60, PEG hydrogenated castor oils 0.46, Na alkyl sulfate solution (27.9 %) 0.75, CuSO4 0.05, glycine 0.03, peppermint flavor 0.24, glycerol 0.15, eugenyl monophosphate 0.15, and vanillyl monophosphate 0.35 %.

PI	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9615768 A1	A1	19960530	WO 1995-US14013	19951027 <--
	W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, UZ, VN				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9540160	A	19960617	AU 1995-40160	19951027 <--
	IN 1995DE02032	A	20050311	IN 1995-DE2032	19951106
	US 5628986	A	19970513	US 1996-632936	19960416 <--
AB	. . . 0.08, ethanol 10.60, PEG hydrogenated castor oils 0.46, Na alkyl sulfate solution (27.9 %) 0.75, CuSO4 0.05, glycine 0.03, peppermint flavor 0.24, glycerol 0.15, eugenyl monophosphate 0.15, and vanillyl monophosphate 0.35 %.				
IT	60-12-8, Benzeneethanol	78-70-6	89-78-1	89-80-5	89-83-8 97-53-0
	100-52-7, Benzaldehyde, biological studies	104-45-0	104-46-1		
	104-55-2	105-54-4	121-32-4	123-33-5	127-41-3 138-86-3
	140-67-0	470-82-6	4422-70-2	4940-11-8	6485-40-1
	RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)				
	(as flavoring agent; antiplaque, antigingivitis dentifrices				

containing phosphates and copper sources)  
 OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS  
 RECORD (13 CITINGS)

PI	WO 9615768 A1	19960530			
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9615768	A1	19960530	WO 1995-US14013	19951027 <--
	W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, UZ, VN				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9540160	A	19960617	AU 1995-40160	19951027 <--
	IN 1995DE02032	A	20050311	IN 1995-DE2032	19951106
	US 5628986	A	19970513	US 1996-632936	19960416 <--

AB Disclosed are oral compns. such as toothpastes, mouth rinses, lozenges, and gums containing at least one phosphate derivative and a copper source. A mouthwash contained water 70.86, sorbitol solution (70 %) 10.25, Na saccharin 0.08, ethanol 10.60, PEG hydrogenated castor oils 0.46, Na alkyl sulfate solution (27.9 %) 0.75, CuSO4 0.05, glycine 0.03, peppermint flavor 0.24, glycerol 0.15, eugenyl monophosphate 0.15, and vanillyl monophosphate 0.35 %.

IT 60-12-8, Benzeneethanol 78-70-6 89-78-1 89-80-5 89-83-8 97-53-0  
 100-52-7, Benzaldehyde, biological studies 104-45-0 104-46-1  
 104-55-2 105-54-4 121-32-4 121-33-5 123-92-2 127-41-3 138-86-3  
 140-67-0 470-82-6 4422-70-2 4940-11-8 6485-40-1  
 RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(as flavoring agent; antiplaque, antigingivitis dentifrices containing phosphates and copper sources)

L29 ANSWER 8 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1996:449693 HCAPLUS

DOCUMENT NUMBER: 125:95620

ORIGINAL REFERENCE NO.: 125:17815a,17818a

TITLE: Antiplaque, antigingivitis oral compositions containing phosphates and copper sources

INVENTOR(S): Sanker, Lowell Alan; Upson, James Grigg

PATENT ASSIGNEE(S): Procter and Gamble Company, USA

SOURCE: PCT Int. Appl., 17 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9615768 A1		19960530	WO 1995-US14013	19951027
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, UZ, VN				
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG				

PRIORITY APPLN. INFO.: US 1994-341716 19941118

ABSTRACT:

Disclosed are oral compns. such as toothpastes, mouthrinses, lozenges, and gums containing at least one phosphate derivative and a copper source. A mouthwash contained water 70.86, sorbitol solution (70 %) 10.25, Na saccharin 0.08, ethanol 10.60, PEG hydrogenated castor oils 0.46, Na alkyl sulfate solution (27.9 %) 0.75, CuSO4 0.05, glycine 0.03, peppermint flavor 0.24, glycerol 0.15, eugenyl

monophosphate 0.15, and vanillyl monophosphate 0.35 %.

PI WO 9615768 A1 19960530

AB . . . 0.08, ethanol 10.60, PEG hydrogenated castor oils 0.46, Na alkyl sulfate solution (27.9 %) 0.75, CuSO<sub>4</sub> 0.05, glycine 0.03, peppermint flavor 0.24, glycerol 0.15, eugenyl monophosphate 0.15, and vanillyl monophosphate 0.35 %.

IT 60-12-8, Phenylethyl alcohol 78-70-6, Linalool 89-78-1, Menthol 89-80-5, Menthone 89-83-8, Thymol 97-53-0, Eugenol 100-52-7, Benzaldehyde, biological studies 104-45-0, Dihydroanethole 104-46-1, Anethole 104-55-2, Cinnamic aldehyde 105-54-4, Ethyl butyrate 121-32-4, Ethyl vanillin 121-33-5, Vanillin 123-92-2, Isoamyl acetate 127-41-3,  $\alpha$ -Ionone 138-86-3, Limonene 140-67-0, Estragole 470-82-6, Eucalyptol 4422-70-2 4940-11-8, Ethylmaltol 6485-40-1  
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(as flavoring agent; antiplaque, antigingivitis dentifrices containing phosphates and copper sources)

PI WO 9615768 A1 19960530

AB Disclosed are oral compns. such as toothpastes, mouthrinses, lozenges, and gums containing at least one phosphate derivative and a copper source. A mouthwash contained water 70.86, sorbitol solution (70 %) 10.25, Na saccharin 0.08, ethanol 10.60, PEG hydrogenated castor oils 0.46, Na alkyl sulfate solution (27.9 %) 0.75, CuSO<sub>4</sub> 0.05, glycine 0.03, peppermint flavor 0.24, glycerol 0.15, eugenyl monophosphate 0.15, and vanillyl monophosphate 0.35 %.

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RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(as flavoring agent; antiplaque, antigingivitis dentifrices containing phosphates and copper sources)

L29 ANSWER 9 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1992:104811 HCAPLUS

DOCUMENT NUMBER: 116:104811

ORIGINAL REFERENCE NO.: 116:17729a,17732a

TITLE: The composition of woodruff volatiles (Galium odoratum)

AUTHOR(S): Woerner, Martin; Schreier, Peter

CORPORATE SOURCE: Univ. Wuerzburg, Wuerzburg, W-8700, Germany

SOURCE: Zeitschrift fuer Lebensmittel-Untersuchung und -Forschung (1991), 193(4), 317-20  
CODEN: ZLUFAR; ISSN: 0044-3026

DOCUMENT TYPE: Journal

LANGUAGE: German

ABSTRACT:

Studies of the composition of an aroma extract of dried woodruff by medium-pressure liquid chromatog. following Soxhlet extraction and chlorophylls removal by gel-permeation chromatog. revealed the presence of 225 substances, 69 of which were alcs., 69 carbonyl compds., 22 hydrocarbons, 20 acids, 19 esters, 14 lactones and 12 other compds. Of the  $\gamma$ -lactones, multi-dimensional gas chromatog. indicated an enantiomeric excess of the R-isomer with increasing chain length. Only 1 substance was previously unknown in nature:

7,11,15-trimethyl-2-hexadecanone; it is thus proposed as an anal. indicator for the detection of the illegal use of woodruff aromas in foods.

SO Zeitschrift fuer Lebensmittel-Untersuchung und -Forschung (1991),  
193(4), 317-20  
CODEN: ZLUFAR; ISSN: 0044-3026

ST woodruff flavor volatile

IT Flavor  
(woodruff, composition of)

IT 57-10-3, Hexadecanoic acid, biological studies 57-11-4, Octadecanoic acid, biological studies 60-12-8, 2-Phenylethanol 64-19-7, Acetic acid, biological studies 65-85-0, Benzoic acid, biological studies 66-25-1, Hexanal 71-36-3, 1-Butanol, biological studies 71-41-0, 1-Pentanol, biological studies 76-22-2 76-49-3, Bornyl acetate 78-36-4 78-70-6, Linalool 78-83-1, 2-Methyl-1-propanol, biological studies 78-92-2, 2-Butanol 78-93-3, 2-Butanone, biological studies 79-77-6,  $\beta$ -Ionone 79-92-5, Camphene 89-80-5, Menthone 89-81-6, Piperitone 89-82-7, Pulegone 89-83-8, Thymol 90-00-6, 2-Ethylphenol 91-64-5, Coumarin 93-15-2, Eugenylmethyl ether 93-55-0, 1-Phenylpropan-1-one 95-48-7, biological studies 98-55-5,  $\alpha$ -Terpineol 99-49-0, Carvone 99-50-3, 3,4-Dihydroxybenzoic acid 99-85-4,  $\gamma$ -Terpinen 99-87-6, p-Cymene 99-93-4, 4-Hydroxyacetophenone 100-51-6, Benzyl alcohol, biological studies 100-52-7, Benzaldehyde, biological studies 103-44-6, 2-Ethylhexylvinyl ether 103-45-7 104-46-1, Anethol 104-76-7, 2-Ethyl-1-hexanol 104-87-0, 4-Methylbenzaldehyde 106-24-1, Geraniol 108-39-4, biological studies 108-95-2, Phenol, biological studies 109-52-4, Pentanoic acid, biological studies 110-15-6, Butanedioic acid, biological studies 110-93-0 111-14-8, Heptanoic acid 111-27-3, 1-Hexanol, biological studies 111-70-6, 1-Heptanol 111-71-7, Heptanal 111-87-5, 1-Octanol, biological studies 112-05-0, Nonanoic acid 112-12-9, 2-Undecanone 112-31-2, Decanal 112-39-0, Methyl hexadecanoate 112-53-8, 1-Dodecanol 112-72-1, 1-Tetradecanol 115-18-4, 2-Methyl-3-buten-2-ol 115-95-7, Linalyl acetate 119-84-6, 3,4-Dihydrocoumarin 122-00-9 123-11-5, 4-Methoxybenzaldehyde, biological studies 123-35-3,  $\beta$ -Myrcene 123-51-3, 3-Methyl-1-butanol 124-07-2, Octanoic acid, biological studies 124-13-0, Octanal 124-19-6, Nonanal 124-25-4, Tetradecanal 124-76-5, Isoborneol 125-12-2, Isobornyl acetate 127-41-3,  $\alpha$ -Ionone 127-91-3,  $\beta$ -Pinene 134-28-1 135-02-4, 2-Methoxybenzaldehyde 140-11-4, Benzyl acetate 141-93-5, 1,3-Diethylbenzene 142-62-1, Hexanoic acid, biological studies 143-07-7, Dodecanoic acid, biological studies 143-08-8, 1-Nonanol 288-13-1, 1H-Pyrazole 334-48-5, Decanoic acid 470-82-6, 1,8-Cineol 471-15-8,  $\beta$ -Thujone 473-06-3, Chrysanthenone 475-03-6, 1,1,6-Trimethyl-1,2,3,4-tetrahydronaphthalene 491-07-6, Isomenthone 497-03-0 499-75-2, Carvacrol 502-69-2, 6,10,14-Trimethyl-2-pentadecanone 505-48-6, Suberic acid 507-70-0, Borneol 515-00-4, Myrtenol 536-60-7, 4-Isopropylbenzyl alcohol 544-63-8, Tetradecanoic acid, biological studies 546-80-5,  $\alpha$ -Thujone 564-94-3, Myrtenal 577-16-2 584-02-1, 3-Pentanol 584-03-2, 1,2-Butanediol 585-74-0 586-62-9, Terpinolene 586-82-3 590-67-0, 1-Methylcyclohexanol 611-14-3, 1-Methyl-2-ethylbenzene 619-62-5 620-14-4, 1-Methyl-3-ethylbenzene 628-46-6, 5-Methylhexanoic acid 628-97-7, Ethyl hexadecanoate 628-99-9, 2-Nonanol 629-11-8, 1,6-Hexanediol 629-80-1, Hexadecanal 629-96-9, 1-Eicosanol 629-99-2, Pentacosane 638-53-9, Tridecanoic acid 693-54-9, 2-Decanone 693-80-1 698-76-0, 8-Octalactone 705-86-2, 8-Decalactone 821-55-6, 2-Nonanone 874-63-5 928-94-9, (Z)-2-Hexen-1-ol 928-95-0, (E)-2-Hexen-1-ol 928-96-1, (Z)-3-Hexen-1-ol 928-97-2, (E)-3-Hexen-1-ol 1002-84-2, Pentadecanoic acid 1070-35-5, Allyl 4-oxopentanoate 1139-30-6, Caryophyllene oxide 1490-04-6, Menthol 1569-50-2,

3-Penten-2-ol 1576-95-0, (Z)-2-Penten-1-ol 1576-96-1,  
 (E)-2-Penten-1-ol 1604-34-8, 6,10-Dimethylundecan-2-one 1653-30-1,  
 2-Undecanol 1669-44-9, 3-Octen-2-one 1678-93-9, Butylcyclohexane  
 1862-61-9 2111-75-3, Perillaaldehyde 2345-27-9, 2-Tetradecanone  
 2345-28-0, 2-Pentadecanone 2408-37-9, 2,2,6-Trimethylcyclohexanone  
 2548-87-0, (E)-2-Octenal 2628-17-3 2867-05-2,  $\alpha$ -Thujene  
 2922-51-2, 2-Heptadecanone 3419-02-1 3623-51-6, Neomenthol  
 3724-65-0, 2-Butenoic acid 3765-28-4 3796-70-1, Geranylacetone  
 3856-25-5,  $\alpha$ -Copaene 4173-41-5 4313-02-4, (E,Z)-2,4-Heptadienal  
 4313-03-5, (E,E)-2,4-Heptadienal 4602-84-0, Farnesol 4630-07-3,  
 Valencene 5273-86-9,  $\beta$ -Asarone 5910-87-2, (E,E)-2,4-Nonadienal  
 5989-33-3 6032-29-7, 2-Pentanol 6175-49-1, 2-Dodecanone 6191-71-5,  
 (Z)-4-Hepten-1-ol 6248-88-0, Fenchene 6728-26-3, (E)-2-Hexenal  
 6728-31-0, (Z)-4-Heptenal 6971-51-3, 3-Methoxybenzyl alcohol  
 7045-71-8, 2-Methylundecane 7149-65-7, Ethyl pyroglutamate 7212-44-4,  
 Nerolidol 7299-42-5,  $\delta$ -Terpineol 7373-13-9, 2-Octadecanone  
 10031-82-0, 4-Ethoxybenzaldehyde 10547-84-9 13466-78-9,  
 A3-Carene 13678-74-5 14009-71-3, (Z)-Linalool oxide pyranoid  
 14398-35-7, 3,4-Didehydro- $\beta$ -ionone 14575-93-0 16303-61-0,  
 2-(5-Methyl-2-furanyl)furan 17092-92-1, Dihydroactinidiolide  
 17699-16-0 18787-63-8, 2-Hexadecanone 18829-55-5, (E)-2-Heptenal  
 18829-56-6, (E)-2-Nonenal 19435-97-3,  $\delta$ -Cadinol 20019-64-1  
 20053-88-7, Hotrienol 20279-49-6, Pentyl 4-oxo-pentanoate 20407-84-5,  
 (E)-2-Dodecanol 22122-36-7, 3-Methyl-2(5H)-furanone 23267-57-4,  
 5,6-Epoxy- $\beta$ -ionone 23313-79-3 23986-74-5, Germacrene D  
 25152-84-5, (E,E)-2,4-Decadienal 28069-72-9 29606-79-9, Isopulegone  
 30086-02-3, (E,E)-3,5-Octadien-2-one 30361-28-5, (E,E)-2,4-Octadienal  
 30364-38-6, 1,1,6-Trimethyl-1,2-dihydronaphthalene 31499-72-6,  
 Dihydro- $\alpha$ -ionone 33081-34-4, Lilac alcohol, a 33081-35-5, Lilac  
 alcohol, b 33393-93-0 34995-77-2 36653-82-4, 1-Hexadecanol  
 38736-62-8 39028-58-5 53448-07-0, (E)-2-Undecenal 54814-64-1  
 55194-06-4 58985-18-5, Dihydroterpinyl acetate 64142-78-5,  
 8-Hydroxylinalool 68922-10-1 72747-25-2, Aromadendrene 97844-14-9  
 137222-06-1 139064-04-3 139113-27-2 139123-06-1 139123-07-2  
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified);  
 BIOL (Biological study); OCCU (Occurrence)

(of woodruff aroma)

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD  
 (3 CITINGS)

SO Zeitschrift fuer Lebensmittel-Untersuchung und -Forschung (1991),  
 193(4), 317-20

CODEN: ZLUFAR; ISSN: 0044-3026

ST woodruff flavor volatile

IT Flavor

(woodruff, composition of)

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 acid, biological studies 60-12-8, 2-Phenylethanol 64-19-7, Acetic  
 acid, biological studies 65-85-0, Benzoic acid, biological studies  
 66-25-1, Hexanal 71-36-3, 1-Butanol, biological studies 71-41-0,  
 1-Pentanol, biological studies 76-22-2 76-49-3, Bornyl acetate  
 78-36-4 78-70-6, Linalool 78-83-1, 2-Methyl-1-propanol, biological  
 studies 78-92-2, 2-Butanol 78-93-3, 2-Butanone, biological studies  
 79-77-6,  $\beta$ -Ionone 79-92-5, Camphene 89-80-5, Menthone 89-81-6,  
 Piperitone 89-82-7, Pulegone 89-83-8, Thymol 90-00-6, 2-Ethylphenol  
 91-64-5, Coumarin 93-15-2, Eugenylmethyl ether 93-55-0,  
 1-Phenylpropan-1-one 95-48-7, biological studies 98-55-5,  
 $\alpha$ -Terpineol 99-49-0, Carvone 99-50-3, 3,4-Dihydroxybenzoic acid  
 99-85-4,  $\gamma$ -Terpinen 99-87-6, p-Cymene 99-93-4,  
 4-Hydroxyacetophenone 100-51-6, Benzyl alcohol, biological studies  
 100-52-7, Benzaldehyde, biological studies 103-44-6, 2-Ethylhexylvinyl  
 ether 103-45-7 104-46-1, Anethol 104-76-7, 2-Ethyl-1-hexanol

104-87-0, 4-Methylbenzaldehyde 106-24-1, Geraniol 108-39-4, biological studies 108-95-2, Phenol, biological studies 109-52-4, Pentanoic acid, biological studies 110-15-6, Butanedioic acid, biological studies 110-93-0 111-14-8, Heptanoic acid 111-27-3, 1-Hexanol, biological studies 111-70-6, 1-Heptanol 111-71-7, Heptanal 111-87-5, 1-Octanol, biological studies 112-05-0, Nonanoic acid 112-12-9, 2-Undecanone 112-31-2, Decanal 112-39-0, Methyl hexadecanoate 112-53-8, 1-Dodecanol 112-72-1, 1-Tetradecanol 115-18-4, 2-Methyl-3-buten-2-ol 115-95-7, Linalyl acetate 119-84-6, 3,4-Dihydrocoumarin 122-00-9 123-11-5, 4-Methoxybenzaldehyde, biological studies 123-35-3,  $\beta$ -Myrcene 123-51-3, 3-Methyl-1-butanol 124-07-2, Octanoic acid, biological studies 124-13-0, Octanal 124-19-6, Nonanal 124-25-4, Tetradecanal 124-76-5, Isoborneol 125-12-2, Isobornyl acetate 127-41-3,  $\alpha$ -Ionone 127-91-3,  $\beta$ -Pinene 134-28-1 135-02-4, 2-Methoxybenzaldehyde 140-11-4, Benzyl acetate 141-93-5, 1,3-Diethylbenzene 142-62-1, Hexanoic acid, biological studies 143-07-7, Dodecanoic acid, biological studies 143-08-8, 1-Nonanol 288-13-1, 1H-Pyrazole 334-48-5, Decanoic acid 470-82-6, 1,8-Cineol 471-15-8,  $\beta$ -Thujone 473-06-3, Chrysanthenone 475-03-6, 1,1,6-Trimethyl-1,2,3,4-tetrahydronaphthalene 491-07-6, Isomenthone 497-03-0 499-75-2, Carvacrol 502-69-2, 6,10,14-Trimethyl-2-pentadecanone 505-48-6, Suberic acid 507-70-0, Borneol 515-00-4, Myrtenol 536-60-7, 4-Isopropylbenzyl alcohol 544-63-8, Tetradecanoic acid, biological studies 546-80-5,  $\alpha$ -Thujone 564-94-3, Myrtenal 577-16-2 584-02-1, 3-Pentanol 584-03-2, 1,2-Butanediol 585-74-0 586-62-9, Terpinolene 586-82-3 590-67-0, 1-Methylcyclohexanol 611-14-3, 1-Methyl-2-ethylbenzene 619-62-5 620-14-4, 1-Methyl-3-ethylbenzene 628-46-6, 5-Methylhexanoic acid 628-97-7, Ethyl hexadecanoate 628-99-9, 2-Nonanol 629-11-8, 1,6-Hexanediol 629-80-1, Hexadecanal 629-96-9, 1-Eicosanol 629-99-2, Pentacosane 638-53-9, Tridecanoic acid 693-54-9, 2-Decanone 693-80-1 698-76-0,  $\delta$ -Octalactone 705-86-2,  $\delta$ -Decalactone 821-55-6, 2-Nonanone 874-63-5 928-94-9, (Z)-2-Hexen-1-ol 928-95-0, (E)-2-Hexen-1-ol 928-96-1, (Z)-3-Hexen-1-ol 928-97-2, (E)-3-Hexen-1-ol 1002-84-2, Pentadecanoic acid 1070-35-5, Allyl 4-oxopentanoate 1139-30-6, Caryophyllene oxide 1490-04-6, Menthol 1569-50-2, 3-Penten-2-ol 1576-95-0, (Z)-2-Penten-1-ol 1576-96-1, (E)-2-Penten-1-ol 1604-34-8, 6,10-Dimethylundecan-2-one 1653-30-1, 2-Undecanol 1669-44-9, 3-Octen-2-one 1678-93-9, Butylcyclohexane 1862-61-9 2111-75-3, Perillaaldehyde 2345-27-9, 2-Tetradecanone 2345-28-0, 2-Pentadecanone 2408-37-9, 2,2,6-Trimethylcyclohexanone 2548-87-0, (E)-2-Octenal 2628-17-3 2867-05-2,  $\alpha$ -Thujene 2922-51-2, 2-Heptadecanone 3419-02-1 3623-51-6, Neomenthol 3724-65-0, 2-Butenoic acid 3765-28-4 3796-70-1, Geranylacetone 3856-25-5,  $\alpha$ -Copaene 4173-41-5 4313-02-4, (E,Z)-2,4-Heptadienal 4313-03-5, (E,E)-2,4-Heptadienal 4602-84-0, Farnesol 4630-07-3, Valencene 5273-86-9,  $\beta$ -Asarone 5910-87-2, (E,E)-2,4-Nonadienal 5989-33-3 6032-29-7, 2-Pentanol 6175-49-1, 2-Dodecanone 6191-71-5, (Z)-4-Hepten-1-ol 6248-88-0, Fenchane 6728-26-3, (E)-2-Hexenal 6728-31-0, (Z)-4-Heptenal 6971-51-3, 3-Methoxybenzyl alcohol 7045-71-8, 2-Methylundecane 7149-65-7, Ethyl pyroglutamate 7212-44-4, Nerolidol 7299-42-5,  $\delta$ -Terpineol 7373-13-9, 2-Octadecanone 10031-82-0, 4-Ethoxybenzaldehyde 10547-84-9 13466-78-9,  $\Delta^3$ -Carene 13678-74-5 14009-71-3, (Z)-Linalool oxide pyranoid 14398-35-7, 3,4-Didehydro- $\beta$ -ionone 14575-93-0 16303-61-0, 2-(5-Methyl-2-furanyl)furan 17092-92-1, Dihydroactinidiolide 17699-16-0 18787-63-8, 2-Hexadecanone 18829-55-5, (E)-2-Heptenal 18829-56-6, (E)-2-Nonenal 19435-97-3,  $\delta$ -Cadinol 20019-64-1, 20053-88-7, Htriolene 20279-49-6, Pentyl 4-oxo-pentanoate 20407-84-5, (E)-2-Dodecenal 22122-36-7, 3-Methyl-2(5H)-furanone 23267-57-4, 5,6-Epoxy- $\beta$ -ionone 23313-79-3 23986-74-5, Germacrene D

25152-84-5, (E,E)-2,4-Decadienal 28069-72-9 29606-79-9, Isopulegone  
 30086-02-3, (E,E)-3,5-Octadien-2-one 30361-28-5, (E,E)-2,4-Octadienal  
 30364-38-6, 1,1,6-Trimethyl-1,2-dihydronaphthalene 31499-72-6,  
 Dihydro- $\alpha$ -ionone 33081-34-4, Lilac alcohol, a 33081-35-5, Lilac  
 alcohol, b 33393-93-0 34995-77-2 36653-82-4, 1-Hexadecanol  
 38736-62-8 39028-58-5 53448-07-0, (E)-2-Undecenal 54814-64-1  
 55194-06-4 58985-18-5, Dihydroterpinyl acetate 64142-78-5,  
 8-Hydroxylinalool 68922-10-1 72747-25-2, Aromadendrene 97844-14-9  
 137222-06-1 139064-04-3 139113-27-2 139123-06-1 139123-07-2  
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified);  
 BIOL (Biological study); OCCU (Occurrence)  
 (of woodruff aroma)

L29 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1990:610224 HCAPLUS

DOCUMENT NUMBER: 113:210224

ORIGINAL REFERENCE NO.: 113:35524h,35525a

TITLE: Characterization of ham flavor using an atomic  
 emission detector

AUTHOR(S): Baloga, David W.; Reineccius, Gary A.; Miller, Joel W.  
 CORPORATE SOURCE: Dep. Food Sci. Nutr., Univ. Minnesota, St. Paul, MN,  
 55108, USA

SOURCE: Journal of Agricultural and Food Chemistry (1990),  
 38(11), 2021-6  
 CODEN: JAFCAU; ISSN: 0021-8561

DOCUMENT TYPE: Journal

LANGUAGE: English

ABSTRACT:

Volatile flavor compds. were isolated from a cured, precooked premium ham by  
 using a Likens-Nickerson apparatus Four individual 250-g ham samples were used to  
 provide flavor isolates, which were pooled and concentrated for extensive gas  
 chromatog. anal. Atomic emission, flame ionization, flame photometry, N-P, and  
 mass spectrometry were used to qual. determine specific constituents of the pooled  
 solvent fraction. At emission were useful in the selective detection of N-,  
 O-, and S-containing compds. More than 60 compds. were tentatively identified,  
 including phenols, aliphatic alcs., ketones, and aldehydes, and cyclooctasulfur.

TI Characterization of ham flavor using an atomic emission detector  
 SO Journal of Agricultural and Food Chemistry (1990), 38(11), 2021-6  
 CODEN: JAFCAU; ISSN: 0021-8561

AB . . . from a cured, precooked premium ham by using a Likens-Nickerson  
 apparatus Four individual 250-g ham samples were used to provide flavor  
 isolates, which were pooled and concentrated for extensive gas chromatog. anal.  
 Atomic emission, flame ionization, flame photometry, N-P, and mass. . .

ST ham flavor analysis; gas chromatog flavor; atomic emission  
 spectrometry flavor

IT Flavor

Odor and Odorous substances

(determination of, of ham by gas chromatog. with atomic emission detection)

IT 66-25-1, Hexanal 78-93-3, 2-Butanone, analysis 84-74-2 90-00-6,  
 2-Ethylphenol 90-05-1 93-51-6, 4-Methylguaiacol 95-48-7, analysis  
 95-65-8 95-87-4 97-53-0, 4-Allylguaiacol 98-01-1,  
 2-Furancarboxaldehyde, analysis 98-86-2, analysis 100-52-7,  
 Benzaldehyde, analysis 105-87-3, Geranyl acetate 106-24-1 106-44-5,  
 analysis 108-39-4, analysis 108-95-2, Phenol, analysis 109-08-0,  
 Methylpyrazine 112-54-9, Dodecanal 121-98-2 122-78-1,  
 Benzeneacetaldehyde 124-25-4, Tetradecanal 128-37-0, analysis  
 135-02-4, 2-Methoxybenzaldehyde 141-78-6, Acetic acid ethyl  
 ester, analysis 150-78-7 526-75-0, 2,3-Dimethylphenol 556-82-1,  
 3-Methyl-2-buten-1-ol 560-21-4, 2,3,3-Trimethylpentane 576-26-1  
 590-86-3 600-14-6, 2,3-Pentanedione 625-74-1, 2-Methyl-1-nitropropane



629-80-1, Hexadecanal 638-66-4, Octadecanal 642-71-7,  
 3,4,5-Trimethoxyphenol 1192-62-7, 2-Acetylfuran 1453-24-3,  
 1-Ethylcyclohexene 1577-52-2, 9,12-Octadecadien-1-ol 1639-04-9,  
 2-Methyl-3-pentanethiol 2345-28-0, 2-Pentadecanone 2758-18-1  
 2765-11-9, Pentadecanal 2785-89-9, 4-Ethylguaiaicol 3581-87-1,  
 2-Methylthiazole 3658-80-8, Dimethyl trisulfide 3877-15-4,  
 1-Methylthiopropene 5090-41-5, 9-Octadecenal 5756-24-1, Dimethyl  
 tetrasulfide 5912-86-7, cis-Isoeugenol 7786-61-0, 4-Vinylguaiaicol  
 10544-50-0, Cyclooctasulfur, analysis 12767-10-1, Octadecadienol  
 26537-70-2, 9,12-Octadecadienal 34314-83-5, 4-Methyl-2,3-dihydrofuran  
 55683-21-1 56554-96-2, 2-Octadecenal 58539-27-8 129216-51-9  
 129216-52-0, 9,17-Octadecadien-1-ol  
 RL: ANT (Analyte); ANST (Analytical study)  
 (determination of, of ham aroma by gas chromatog. with atomic emission  
 detector)

OS.CITING REF COUNT: 12 THERE ARE 12 CAPLUS RECORDS THAT CITE THIS  
 RECORD (12 CITINGS)

TI Characterization of ham flavor using an atomic emission detector  
 SO Journal of Agricultural and Food Chemistry (1990), 38(11), 2021-6  
 CODEN: JAFCAU; ISSN: 0021-8561

AB Volatile flavor compds. were isolated from a cured, precooked premium ham  
 by using a Likens-Nickerson apparatus Four individual 250-g ham samples were  
 used to provide flavor isolates, which were pooled and concentrated for  
 extensive gas chromatog. anal. Atomic emission, flame ionization, flame  
 photometry, N-P, and mass spectrometry were used to qual. determine specific  
 constituents of the pooled solvent fraction. At emission were useful in  
 the selective detection of N-, O-, and S-containing compds. More than 60  
 compds. were tentatively identified, including phenols, aliphatic alcs.,  
 ketones, and aldehydes, and cyclooctasulfur.

ST ham flavor analysis; gas chromatog flavor; atomic emission  
 spectrometry flavor

IT Flavor  
 Odor and Odorous substances

(determination of, of ham by gas chromatog. with atomic emission detection)  
 IT 66-25-1, Hexanal 78-93-3, 2-Butanone, analysis 84-74-2 90-00-6,  
 2-Ethylphenol 90-05-1 93-51-6, 4-Methylguaiaicol 95-48-7, analysis  
 95-65-8 95-87-4 97-53-0, 4-Allylguaiaicol 98-01-1,  
 2-Furancarboxaldehyde, analysis 98-86-2, analysis 100-52-7,  
 Benzaldehyde, analysis 105-87-3, Geranyl acetate 106-24-1 106-44-5,  
 analysis 108-39-4, analysis 108-95-2, Phenol, analysis 109-08-0,  
 Methylpyrazine 112-54-9, Dodecanal 121-98-2 122-78-1,  
 Benzeneacetaldehyde 124-25-4, Tetradecanal 128-37-0, analysis  
 135-02-4, 2-Methoxybenzaldehyde 141-78-6, Acetic acid ethyl  
 ester, analysis 150-78-7 526-75-0, 2,3-Dimethylphenol 556-82-1,  
 3-Methyl-2-buten-1-ol 560-21-4, 2,3,3-Trimethylpentane 576-26-1  
 590-86-3 600-14-6, 2,3-Pentanedione 625-74-1, 2-Methyl-1-nitropropane  
 629-80-1, Hexadecanal 638-66-4, Octadecanal 642-71-7,  
 3,4,5-Trimethoxyphenol 1192-62-7, 2-Acetylfuran 1453-24-3,  
 1-Ethylcyclohexene 1577-52-2, 9,12-Octadecadien-1-ol 1639-04-9,  
 2-Methyl-3-pentanethiol 2345-28-0, 2-Pentadecanone 2758-18-1  
 2765-11-9, Pentadecanal 2785-89-9, 4-Ethylguaiaicol 3581-87-1,  
 2-Methylthiazole 3658-80-8, Dimethyl trisulfide 3877-15-4,  
 1-Methylthiopropene 5090-41-5, 9-Octadecenal 5756-24-1, Dimethyl  
 tetrasulfide 5912-86-7, cis-Isoeugenol 7786-61-0, 4-Vinylguaiaicol  
 10544-50-0, Cyclooctasulfur, analysis 12767-10-1, Octadecadienol  
 26537-70-2, 9,12-Octadecadienal 34314-83-5, 4-Methyl-2,3-dihydrofuran  
 55683-21-1 56554-96-2, 2-Octadecenal 58539-27-8 129216-51-9  
 129216-52-0, 9,17-Octadecadien-1-ol

RL: ANT (Analyte); ANST (Analytical study)  
 (determination of, of ham aroma by gas chromatog. with atomic emission  
 detector)

L29 ANSWER 11 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1989:630914 HCAPLUS

DOCUMENT NUMBER: 111:230914

ORIGINAL REFERENCE NO.: 111:38361a,38364a

TITLE: Styrene production by *Penicillium camemberti* Thom

AUTHOR(S): Adda, J.; Dekimpe, J.; Vassal, L.; Spinnler, H. E.

CORPORATE SOURCE: Lab. Rech. Aromes, INRA, Dijon, Fr.

SOURCE: Lait (1989), 69(2), 115-20

CODEN: LAITAG; ISSN: 0023-7302

DOCUMENT TYPE: Journal

LANGUAGE: French

ABSTRACT:

The celluloid taste observed in some mold-ripened cheeses is related to the presence of styrene in these cheeses. The accumulation of this mol. was only detected on cultures of some strains of *Penicillium camemberti*. It seems to be related to a change in oxidative metabolism in these strains. Volatile products of soft mold-ripened cheeses were examined by capillary gas chromatog.

SO Lait (1989), 69(2), 115-20

CODEN: LAITAG; ISSN: 0023-7302

ST *Penicillium* styrene cheese flavor; soft cheese flavor styrene

IT *Penicillium camemberti*

(styrene formation by, cheese off-flavor in relation to)

IT Flavor

(off-, of mold-ripened soft cheese, styrene formation by *Penicillium camemberti* in relation to)

IT Cheese

(soft, flavor of mold-ripened, *Penicillium camemberti* styrene formation)

IT 54-11-5, Nicotine 60-12-8, Phenyl-2-ethanol 67-71-0, Dimethyl sulfone

71-41-0, Pentanol, biological studies 87-44-5 91-20-3, Naphthalene,

biological studies 96-17-3, Methyl-2-butanal 98-55-5,

$\alpha$ -Terpineol 100-52-7, Benzaldehyde, biological studies 100-66-3,

Methoxybenzene, biological studies 105-54-4, Ethyl butyrate 106-32-1

106-68-3, 3-Octanone 107-87-9, 2-Pentanone 108-88-3, Toluene,

biological studies 110-38-3, Ethyl decanoate 110-43-0, Heptan-2-one

111-13-7, Octan-2-one 111-27-3, Hexanol, biological studies 111-87-5,

Octan-1-ol, biological studies 112-12-9, Undecan-2-one 112-30-1,

Decan-1-ol 112-53-8, Dodecanol 120-72-9, 1H-Indole, biological studies

123-51-3, Methyl-3-butan-1-ol 124-19-6, Nonanal 128-37-0, BHT,

biological studies 140-29-4, Benzylcyanide 151-10-0,

1,3-Dimethoxybenzene 589-98-0, Octan-3-ol 591-78-6, Hexan-2-one

593-08-8, Tridecan-2-one 624-92-0, Dimethyldisulfide 628-99-9,

Nonan-2-ol 693-54-9, Decan-2-one 821-55-6, Nonan-2-one 1330-20-7,

Xylene, biological studies 1484-17-9, Ethyl S-thiobenzoate 1653-30-1,

Undecan-2-ol 3391-86-4, Oct-1-en-3-ol 6032-29-7, Pentan-2-ol

7380-48-5, Oct-3-enyl acetate 20013-10-9, Non-8-en-3-one 25321-22-6,

Dichlorobenzene 25550-14-5, Ethyl methyl benzene 27323-28-0, Methyl

indole 27936-14-7, Undecen-2-one 57782-14-6, Tridecenone 69093-74-9,

Dec-3-en-1-ol 83861-74-9, Octa-1,5-dien-3-ol

RL: BIOL (Biological study)

(of mold-ripened soft cheese aroma)

IT 100-42-5, biological studies

RL: BIOL (Biological study)

(of mold-ripened soft cheese off-flavor, *Penicillium camemberti* formation of)

OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS

RECORD (13 CITINGS)

SO Lait (1989), 69(2), 115-20

CODEN: LAITAG; ISSN: 0023-7302

ST Penicillium styrene cheese flavor; soft cheese flavor styrene  
 IT Penicillium camembertii  
 (styrene formation by, cheese off-flavor in relation to)  
 IT Flavor  
 (off-, of mold-ripened soft cheese, styrene formation by Penicillium  
 camemberti in relation to)  
 IT Cheese  
 (soft, flavor of mold-ripened, Penicillium camemberti styrene  
 formation)  
 IT 54-11-5, Nicotine 60-12-8, Phenyl-2-ethanol 67-71-0, Dimethyl sulfone  
 71-41-0, Pentanol, biological studies 87-44-5 91-20-3, Naphthalene,  
 biological studies 96-17-3, Methyl-2-butanal 98-55-5,  
 $\alpha$ -Terpineol 100-52-7, Benzaldehyde, biological studies 100-66-3,  
 Methoxybenzene, biological studies 105-54-4, Ethyl butyrate 106-32-1  
 106-68-3, 3-Octanone 107-87-9, 2-Pentanone 108-88-3, Toluene,  
 biological studies 110-38-3, Ethyl decanoate 110-43-0, Heptan-2-one  
 111-13-7, Octan-2-one 111-27-3, Hexanol, biological studies 111-87-5,  
 Octan-1-ol, biological studies 112-12-9, Undecan-2-one 112-30-1,  
 Decan-1-ol 112-53-8, Dodecanol 120-72-9, 1H-Indole, biological studies  
 123-51-3, Methyl-3-butan-1-ol 124-19-6, Nonanal 128-37-0, BHT,  
 biological studies 140-29-4, Benzylcyanide 151-10-0,  
 1,3-Dimethoxybenzene 589-98-0, Octan-3-ol 591-78-6, Hexan-2-one  
 593-08-8, Tridecan-2-one 624-92-0, Dimethyldisulfide 628-99-9,  
 Nonan-2-ol 693-54-9, Decan-2-one 821-55-6, Nonan-2-one 1330-20-7,  
 Xylene, biological studies 1484-17-9, Ethyl S-thiobenzoate 1653-30-1,  
 Undecan-2-ol 3391-86-4, Oct-1-en-3-ol 6032-29-7, Pentan-2-ol  
 7380-48-5, Oct-3-enyl acetate 20013-10-9, Non-8-en-3-one 25321-22-6,  
 Dichlorobenzene 25550-14-5, Ethyl methyl benzene 27323-28-0, Methyl  
 indole 27936-14-7, Undecen-2-one 57782-14-6, Tridecenone 69093-74-9,  
 Dec-3-en-1-ol 83861-74-9, Octa-1,5-dien-3-ol  
 RL: BIOL (Biological study)  
 (of mold-ripened soft cheese aroma)  
 IT 100-42-5, biological studies  
 RL: BIOL (Biological study)  
 (of mold-ripened soft cheese off-flavor, Penicillium  
 camemberti formation of)

L29 ANSWER 12 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1988:20686 HCAPLUS

DOCUMENT NUMBER: 108:20686

ORIGINAL REFERENCE NO.: 108:3501a,3504a

TITLE: The metabolic disposition of [methoxy-14C]-labeled  
 trans-anethole, estragole and p-propylanisole in human  
 volunteers

AUTHOR(S): Sangster, Susan A.; Caldwell, John; Hutt, Andrew J.;

Anthony, Andrew; Smith, Robert L.

CORPORATE SOURCE: Med. Sch., St. Mary's Hosp., London, W2 1PG, UK

SOURCE: Xenobiotica (1987), 17(10), 1223-32

CODEN: XENOBH; ISSN: 0049-8254

DOCUMENT TYPE: Journal

LANGUAGE: English

ABSTRACT:

The metabolic fates of the naturally occurring food flavors trans-anethole  
 and estragole, and their synthetic congener p-propylanisole, were investigated  
 in human volunteers by using the [methoxy-14C]-labeled compds. The doses used  
 were close to those encountered in the diet, 1 mg, 100  $\mu$ g, and 100  $\mu$ g  
 resp. In each case, the major routes of elimination of 14C were in the urine  
 and in the expired air as 14CO<sub>2</sub>. Urinary metabolites were separated by solvent  
 extraction, TLC and HPLC, and characterized by comparison of chromatog. mobilities  
 with stds. and by radioisotope dilution. Nine 14C urinary metabolites were found  
 after trans-anethole administration, 4 after p-propylanisole, and 5 after

estragole. All were products of side-chain oxidns. The principal metabolites of p-propylanisole were 4-methoxyhippuric acid (12%) and 1-(4'-methoxyphenyl)propan-1-ol (2%) and -2-ol (8%). The major metabolite of trans-anethole was 4-methoxyhippuric acid (56% of dose), accompanied by much smaller amts. of the 2 isomers of 1-(4'-methoxyphenyl)propane-1,2-diol (together 3%). After estragole administration, the 2 volunteers eliminated 0.2 and 0.4% of the dose, resp., as 1'-hydroxyestragole. The human metabolic data is discussed with reference to the comparative metabolic disposition of these compds. in the mouse and rat, species commonly used for safety assessment.

SO Xenobiotica (1987), 17(10), 1223-32  
CODEN: XENOBH; ISSN: 0049-8254

AB The metabolic fates of the naturally occurring food flavors trans-anethole and estragole, and their synthetic congener p-propylanisole, were investigated in human volunteers by using the [methoxy-14C]-labeled compds. The doses. . .

IT Flavor

(anethole and estragole of, metabolism of, in humans)

IT Flavoring materials

(propylanisol of, metabolism of, in humans)

IT 104-45-0, p-Propylanisole 140-67-0, Estragole 4180-23-8,  
trans-Anethole

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(metabolism of, in humans, food flavor use in relation to)

IT 5349-60-0

RL: BIOL (Biological study)

(propylanisole flavoring metabolite, in humans)

OS.CITING REF COUNT: 34 THERE ARE 34 CAPLUS RECORDS THAT CITE THIS  
RECORD (34 CITINGS)

SO Xenobiotica (1987), 17(10), 1223-32  
CODEN: XENOBH; ISSN: 0049-8254

AB The metabolic fates of the naturally occurring food flavors trans-anethole and estragole, and their synthetic congener p-propylanisole, were investigated in human volunteers by using the [methoxy-14C]-labeled compds. The doses used were close to those encountered in the diet, 1 mg, 100 µg, and 100 µg resp. In each case, the major routes of elimination of 14C were in the urine and in the expired air as 14CO2. Urinary metabolites were separated by solvent extraction,

TLC and HPLC, and characterized by comparison of chromatog. mobilities with stds. and by radioisotope dilution. Nine 14C urinary metabolites were found after trans-anethole administration, 4 after p-propylanisole, and 5 after estragole. All were products of side-chain oxidns. The principal metabolites of p-propylanisole were 4-methoxyhippuric acid (12%) and 1-(4'-methoxyphenyl)propan-1-ol (2%) and -2-ol (8%). The major metabolite of trans-anethole was 4-methoxyhippuric acid (56% of dose), accompanied by much smaller amts. of the 2 isomers of 1-(4'-methoxyphenyl)propane-1,2-diol (together 3%). After estragole administration, the 2 volunteers eliminated 0.2 and 0.4% of the dose, resp., as 1'-hydroxyestragole. The human metabolic data is discussed with reference to the comparative metabolic disposition of these compds. in the mouse and rat, species commonly used for safety assessment.

IT Flavor

(anethole and estragole of, metabolism of, in humans)

IT Flavoring materials

(propylanisol of, metabolism of, in humans)

IT 104-45-0, p-Propylanisole 140-67-0, Estragole 4180-23-8,  
trans-Anethole

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(metabolism of, in humans, food flavor use in relation to)  
IT 5349-60-0  
RL: BIOL (Biological study)  
(propylanisole flavoring metabolite, in humans)

L29 ANSWER 13 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1985:130580 HCAPLUS  
DOCUMENT NUMBER: 102:130580  
ORIGINAL REFERENCE NO.: 102:20477a,20480a  
TITLE: Consumption ratio and food predominance of flavoring materials - second cumulative series  
AUTHOR(S): Stofberg, Jan; Grundschober, Friedrich  
CORPORATE SOURCE: PFW, Div., Hercules Inc., Middletown, NY, 10940, USA  
SOURCE: Perfumer & Flavorist (1984), 9(4), 53-6, 58-9, 62, 65-72, 76-83  
CODEN: PEFLDI; ISSN: 0361-8587  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
ABSTRACT:

Detailed data are tabulated on the consumption ratio of food flavoring materials, i.e., the ratio between the quantity of a flavoring material consumed as an ingredient of food and the quantity of the same flavorant consumed as a component of added flavoring material. The food consumption ratio was calculated from the USA literature data published after 1983. Of 347 flavoring materials covered, 296 were found as food predominant or those having the consumption ratio of >1; 205 of them had a consumption ratio of >10.

TI Consumption ratio and food predominance of flavoring materials - second cumulative series  
SO Perfumer & Flavorist (1984), 9(4), 53-6, 58-9, 62, 65-72, 76-83  
CODEN: PEFLDI; ISSN: 0361-8587  
AB Detailed data are tabulated on the consumption ratio of food flavoring materials, i.e., the ratio between the quantity of a flavoring material consumed as an ingredient of food and the quantity of the same flavorant consumed as a component of added flavoring material. The food consumption ratio was calculated from the USA literature data published after 1983. Of 347 flavoring materials covered, 296 were found as food predominant or those having the consumption ratio of >1; 205 of them had.

ST flavoring material food diet

IT Flavoring materials  
(food consumption ratio of)

IT 57-06-7 57-10-3, biological studies 57-11-4, biological studies  
60-12-8 60-33-3, biological studies 64-18-6, biological studies  
66-25-1 67-63-0, biological studies 67-64-1, biological studies  
71-23-8, biological studies 71-36-3, biological studies 71-41-0,  
biological studies 74-93-1, biological studies 75-07-0, biological  
studies 75-18-3 76-49-3 78-70-6 78-83-1, biological studies  
78-84-2 78-92-2 78-93-3, biological studies 78-98-8 79-09-4,  
biological studies 79-20-9 79-31-2 79-76-5 79-77-6 79-82-5  
80-56-8 80-71-7 83-34-1 87-44-5 90-02-8, biological studies  
90-05-1 90-12-0 92-52-4, biological studies 93-15-2 93-16-3  
93-51-6 93-58-3 93-89-0 94-46-2 95-48-7, biological studies  
95-65-8 95-87-4 96-17-3 96-48-0 97-54-1 97-62-1 97-87-0  
98-00-0 98-01-1, biological studies 98-02-2 98-55-5 98-85-1  
98-86-2, biological studies 99-83-2 99-85-4 99-86-5 99-87-6  
100-42-5, biological studies 100-51-6, biological studies 100-52-7,  
biological studies 103-36-6 103-45-7 103-95-7 104-09-6 104-50-7  
104-57-4 104-61-0 104-67-6 104-76-7 105-21-5 105-37-3 105-54-4  
105-68-0 105-79-3 105-87-3 106-18-3 106-21-8 106-22-9 106-23-0

106-24-1	106-25-2	106-27-4	106-29-6	106-30-9	106-32-1	106-33-2
106-35-4	106-36-5	106-44-5, biological studies	106-70-7	107-85-7		
107-87-9	107-92-6, biological studies	108-10-1	108-29-2	108-39-4, biological studies		
109-08-0	109-19-3	109-21-7	109-52-4, biological studies	109-60-4		
109-94-4	109-97-7	110-19-0	110-38-3	110-39-4	110-43-0	110-62-3
110-86-1, biological studies			110-89-4, biological studies	110-93-0		
111-11-5	111-13-7	111-14-8	111-27-3, biological studies	111-70-6		
111-82-0	111-87-5, biological studies	112-05-0	112-06-1	112-12-9		
112-14-1	112-17-4	112-30-1	112-31-2	112-37-8	112-54-9	
112-80-1, biological studies		115-95-7	118-71-8	119-36-8	120-72-9, biological studies	
123-19-3	123-25-1	123-32-0	123-35-3	123-38-6, biological studies		
123-51-3	123-66-0	123-72-8	123-75-1, biological studies	123-92-2		
123-96-6	124-06-1	124-07-2, biological studies	124-10-7	124-13-0		
124-19-6	127-41-3	127-91-3	138-87-4	140-11-4	140-26-1	140-88-5
141-12-8	141-14-0	141-16-2	141-78-6, biological studies	141-97-9		
142-50-7	142-62-1, biological studies	143-13-5	150-84-5	431-03-8	463-40-1	464-49-3
470-82-6	488-10-8	491-04-3	491-09-8	495-62-5	497-03-0	499-75-2
503-74-2	505-10-2	505-57-7	507-70-0	513-86-0	540-07-8	540-18-1
542-55-2	543-49-7	544-12-7	544-63-8, biological studies	546-79-2		
547-63-7	556-24-1	556-82-1	557-48-2	562-74-3	576-26-1	
582-24-1	586-62-9	589-38-8	589-98-0	590-01-2	590-86-3	
592-84-7	593-08-8	600-14-6	606-45-1	616-25-1	620-02-0	623-17-6
623-19-8	623-36-9	623-42-7	623-70-1	624-24-8	624-92-0	626-77-7
626-82-4	628-99-9	629-19-6	638-11-9	638-25-5	695-06-7	698-76-0
705-86-2	706-14-9	710-04-3	713-95-1	764-39-6		

RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)  
(flavorant, food consumption ratio of)

IT	821-55-6	823-22-3	870-23-5	1072-83-9	1117-52-8	1117-55-1
	1122-62-9	1124-11-4	1139-30-6	1192-62-7	1193-79-9	1365-19-1
	1438-94-4	1632-73-1	2035-99-6	2050-01-3	2111-75-3	2198-61-0
	2305-05-7	2305-21-7	2345-26-8	2349-07-7	2363-89-5	2412-80-8
	2463-53-8	2463-77-6	2497-18-9	2639-63-6	2721-22-4	2785-89-9
	3025-30-7	3142-66-3	3188-00-9	3268-49-3	3301-94-8	3391-86-4
	3658-77-3	3658-80-8	3777-69-3	3796-70-1	3848-24-6	3913-71-1
	4411-89-6	4437-22-3	4630-07-3	4674-50-4	5392-40-5	5454-09-1
	5454-28-4	5457-70-5	5905-46-4	5905-47-5	5910-85-0	5910-89-4
	5989-27-5	6028-61-1	6032-29-7	6290-37-5	6309-51-9	6378-65-0
	6380-23-0	6789-80-6	6946-90-3	7452-79-1	7786-44-9	7786-61-0
	10032-15-2	13162-46-4	13327-56-5	13360-64-0	13360-65-1	
	13532-18-8	13623-11-5	13679-46-4	13679-85-1	13925-00-3	
	13925-06-9	13925-07-0	13925-08-1	14667-55-1	15706-73-7	
	15707-23-0	16409-46-4	17619-36-2	18640-74-9	18829-55-5	
	21188-58-9	21834-92-4	22047-25-2	23328-62-3	23726-93-4	
	24295-03-2	25152-84-5	29811-50-5	31501-11-8	35854-86-5	
	40228-18-0	56747-96-7	57500-00-2	59094-77-8	62238-34-0	
	65505-17-1	76649-16-6	79869-58-2	93905-03-4	94280-80-5	

RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)  
(flavorant, food consumption ratio of)

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD  
(2 CITINGS)

TI Consumption ratio and food predominance of flavoring materials - second cumulative series

SO Perfumer & Flavorist ( 1984), 9(4), 53-6, 58-9, 62, 65-72, 76-83  
CODEN: PEFLDI; ISSN: 0361-8587

AB Detailed data are tabulated on the consumption ratio of food flavoring materials, i.e., the ratio between the quantity of a flavoring material consumed as an ingredient of food and the quantity of the same flavorant consumed as a component of added flavoring material. The food

consumption ratio was calculated from the USA literature data published after 1983. Of 347 flavoring materials covered, 296 were found as food predominant or those having the consumption ratio of >1; 205 of them had a consumption ratio of >10.

ST flavoring material food diet

IT Flavoring materials

(food consumption ratio of)

IT	57-06-7	57-10-3, biological studies	57-11-4, biological studies
	60-12-8	60-33-3, biological studies	64-18-6, biological studies
	66-25-1	67-63-0, biological studies	67-64-1, biological studies
	71-23-8, biological studies	71-36-3, biological studies	71-41-0, biological studies
	74-93-1, biological studies	75-07-0, biological studies	75-18-3, biological studies
	76-49-3	78-70-6	78-83-1, biological studies
	78-84-2	78-92-2	78-93-3, biological studies
	79-20-9	79-31-2	79-76-5
	80-56-8	80-71-7	83-34-1
	87-44-5	90-02-8, biological studies	93-15-2
	90-05-1	90-12-0	92-52-4, biological studies
	93-51-6	93-58-3	93-89-0
	95-65-8	95-87-4	96-17-3
	96-48-0	97-54-1	97-62-1
	97-87-0	98-00-0	98-01-1, biological studies
	98-02-2	98-55-5	98-85-1
	98-86-2, biological studies	99-83-2	99-85-4
	99-86-5	99-87-6	100-42-5, biological studies
	100-51-6, biological studies	100-52-7, biological studies	103-36-6
	103-45-7	103-95-7	104-09-6
	104-57-4	104-61-0	104-67-6
	104-76-7	105-21-5	105-37-3
	105-54-4	105-68-0	105-79-3
	105-87-3	106-18-3	106-21-8
	106-22-9	106-24-1	106-25-2
	106-27-4	106-29-6	106-30-9
	106-32-1	106-33-2	106-35-4
	106-36-5	106-44-5, biological studies	106-70-7
	107-85-7	107-92-6, biological studies	108-10-1
	108-29-2	108-39-4, biological studies	108-50-9
	108-64-5	108-95-2, biological studies	109-08-0
	109-19-3	109-21-7	109-52-4, biological studies
	109-60-4	109-94-4	109-97-7
	110-19-0	110-38-3	110-39-4
	110-43-0	110-62-3	110-86-1, biological studies
	110-89-4, biological studies	110-93-0	111-11-5
	111-13-7	111-14-8	111-27-3, biological studies
	111-70-6	111-82-0	111-87-5, biological studies
	112-05-0	112-06-1	112-12-9
	112-14-1	112-17-4	112-30-1
	112-31-2	112-37-8	112-54-9
	112-80-1, biological studies	115-95-7	118-71-8
	119-36-8	120-72-9, biological studies	121-33-5
	122-70-3	122-72-5	122-78-1
	123-07-9	123-19-3	123-25-1
	123-32-0	123-35-3	123-38-6, biological studies
	123-51-3	123-66-0	123-72-8
	123-75-1, biological studies	123-92-2	123-96-6
	124-06-1	124-07-2, biological studies	124-10-7
	124-13-0	124-19-6	127-41-3
	127-91-3	138-87-4	140-11-4
	140-26-1	140-88-5	141-12-8
	141-14-0	141-16-2	141-78-6, biological studies
	141-97-9	142-50-7	142-62-1, biological studies
	142-92-7	143-07-7, biological studies	143-08-8
	143-13-5	150-84-5	431-03-8
	463-40-1	464-49-3	470-82-6
	488-10-8	491-04-3	491-09-8
	495-62-5	497-03-0	499-75-2
	503-74-2	505-10-2	505-57-7
	507-70-0	513-86-0	540-07-8
	540-18-1	542-55-2	543-49-7
	544-12-7	544-63-8, biological studies	546-79-2
	547-63-7	556-24-1	556-82-1
	557-48-2	562-74-3	576-26-1
	582-24-1	586-62-9	589-38-8
	589-98-0	590-01-2	590-86-3
	592-84-7	593-08-8	600-14-6
	606-45-1	616-25-1	620-02-0
	623-19-8	623-36-9	623-42-7
	623-70-1	624-24-8	624-92-0
	626-82-4	628-99-9	629-19-6
	638-11-9	638-25-5	695-06-7
	698-76-0	705-86-2	706-14-9
	710-04-3	713-95-1	764-39-6
RL:	FFD (Food or feed use); BIOL (Biological study); USES (Uses)		
	(flavorant, food consumption ratio of)		
IT	821-55-6	823-22-3	870-23-5
	1072-83-9	1117-52-8	1117-55-1
	1122-62-9	1124-11-4	1139-30-6
	1192-62-7	1193-79-9	1365-19-1
	1438-94-4	1632-73-1	2035-99-6
	2050-01-3	2111-75-3	2198-61-0
	2305-05-7	2305-21-7	2345-26-8
	2349-07-7	2363-89-5	2412-80-8
	2463-53-8	2463-77-6	2497-18-9
	2639-63-6	2721-22-4	2785-89-9
	3025-30-7	3142-66-3	3188-00-9
	3268-49-3	3301-94-8	3391-86-4

3658-77-3	3658-80-8	3777-69-3	3796-70-1	3848-24-6	3913-71-1
4411-89-6	4437-22-3	4630-07-3	4674-50-4	5392-40-5	5454-09-1
5454-28-4	5457-70-5	5905-46-4	5905-47-5	5910-85-0	5910-89-4
5989-27-5	6028-61-1	6032-29-7	6290-37-5	6309-51-9	6378-65-0
6380-23-0	6789-80-6	6946-90-3	7452-79-1	7786-44-9	7786-61-0
10032-15-2	13162-46-4	13327-56-5	13360-64-0	13360-65-1	
13532-18-8	13623-11-5	13679-46-4	13679-85-1	13925-00-3	
13925-06-9	13925-07-0	13925-08-1	14667-55-1	15706-73-7	
15707-23-0	16409-46-4	17619-36-2	18640-74-9	18829-55-5	
21188-58-9	21834-92-4	22047-25-2	23328-62-3	23726-93-4	
24295-03-2	25152-84-5	29811-50-5	31501-11-8	35854-86-5	
40228-18-0	56747-96-7	57500-00-2	59094-77-8	62238-34-0	
65505-17-1	76649-16-6	79869-58-2	93905-03-4	94280-80-5	

RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)  
(flavorant, food consumption ratio of)

L29 ANSWER 14 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1985:44486 HCAPLUS

DOCUMENT NUMBER: 102:44486

ORIGINAL REFERENCE NO.: 102:6987a,6990a

TITLE: A case of artefact formation when using hydrogen as carrier gas in capillary gas chromatography

AUTHOR(S): Liddle, P. A. P.; Bossard, A.

CORPORATE SOURCE: Martini and Rossi, Saint-Ouen, 93401, Fr.

SOURCE: HRC & CC, Journal of High

Resolution Chromatography

and Chromatography Communications (1984), 7(11), 646-7

CODEN: HCJCDB; ISSN: 0344-7138

DOCUMENT TYPE: Journal

LANGUAGE: English

ABSTRACT:

A small amount (5%) of anethole [104-46-1] was converted to dihydroanethole [104-45-0] during its separation by gas chromatog. on a capillary Carbowax 20M column with H as the carrier gas. The implications of this finding for the determination of flavor volatiles by gas chromatog. are discussed.

SO HRC & CC, Journal of High Resolution Chromatography and Chromatography Communications (1984), 7(11), 646-7  
CODEN: HCJCDB; ISSN: 0344-7138

AB . . . a capillary Carbowax 20M column with H as the carrier gas. The implications of this finding for the determination of flavor volatiles by gas chromatog. are discussed.

IT Hydrogenation  
(of anethole, in gas chromatog., flavor compound determination in relation to)

IT 104-45-0  
RL: FORM (Formation, nonpreparative)  
(formation of, in anethole determination by gas chromatog., flavor compound determination in relation to)

IT 104-46-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(hydrogenation of, in gas chromatog., flavor compound determination in relation to)

SO HRC & CC, Journal of High Resolution Chromatography and Chromatography Communications (1984), 7(11), 646-7  
CODEN: HCJCDB; ISSN: 0344-7138

AB A small amount (5%) of anethole [104-46-1] was converted to dihydroanethole [104-45-0] during its separation by gas chromatog. on a capillary Carbowax 20M column with H as the carrier gas. The implications of this finding for the determination of flavor volatiles by gas chromatog. are discussed.



IT Hydrogenation  
(of anethole, in gas chromatog., flavor compound determination in relation to)  
IT 104-45-0  
RL: FORM (Formation, nonpreparative)  
(formation of, in anethole determination by gas chromatog., flavor compound determination in relation to)  
IT 104-46-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(hydrogenation of, in gas chromatog., flavor compound determination in relation to)

L29 ANSWER 15 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1984:119500 HCAPLUS

DOCUMENT NUMBER: 100:119500

ORIGINAL REFERENCE NO.: 100:18161a,18164a

TITLE: Study of artificial flavoring substances for mutagenicity in the Salmonella/microsome, Basc and micronucleus tests

AUTHOR(S): Wild, D.; King, M. T.; Gocke, E.; Eckhardt, K.

CORPORATE SOURCE: Zentrallab. Mutagenitaetspruef., Dtsch.

Forschungsgemeinsch., Freiburg, D-7800, Fed. Rep. Ger.

SOURCE: Food and Chemical Toxicology (1983), 21(6), 707-19

CODEN: FCTOD7; ISSN: 0278-6915

DOCUMENT TYPE: Journal

LANGUAGE: English

ABSTRACT:

Seventy-six compds. used as artificial flavoring substances in food products were studied for mutagenic properties by the use of the Salmonella/mammalian microsome test (Ames test), Basc test on Drosophila melanogaster, and micronucleus test on mouse bone marrow. The following 4 compds. were mutagenic in Ames tests. EtNO2 [109-95-5], ethyl 3-phenylglycidate [121-39-1], 6-methylquinoline [91-62-3] and musk ambrette. Of these EtNO2 and musk ambrette also induced an increase in sex-linked recessive lethal mutations in Drosophila. Two further compds. ethyl 3-methyl-3-phenylglycidate [77-83-8] and 4-propylanisole [104-45-0], appeared weakly mutagenic in Drosophila only. The result with 4-propylanisole was of equivocal biol. significance. None of the flavoring substances induced micronuclei, i.e. cytogenetic damage in the bone marrow of mice.

TI Study of artificial flavoring substances for mutagenicity in the Salmonella/microsome, Basc and micronucleus tests

SO Food and Chemical Toxicology (1983), 21(6), 707-19

CODEN: FCTOD7; ISSN: 0278-6915

AB Seventy-six compds. used as artificial flavoring substances in food products were studied for mutagenic properties by the use of the Salmonella/mammalian microsome test (Ames test), Basc. . . 4-propylanisole [104-45-0], appeared weakly mutagenic in Drosophila only. The result with 4-propylanisole was of equivocal biol. significance. None of the flavoring substances induced micronuclei, i.e. cytogenetic damage in the bone marrow of mice.

ST flavoring material mutagenicity

IT Mutagens

(flavoring materials)

IT Flavoring materials

(mutagenicity of)

IT 77-83-8 91-62-3 104-45-0 109-95-5 121-39-1

RL: ADV (Adverse effect, including toxicity); FFD (Food or feed use); BIOL (Biological study); USES (Uses)

(flavoring material, mutagenicity of)

OS.CITING REF COUNT: 62 THERE ARE 62 CAPLUS RECORDS THAT CITE THIS

# RECORD (62 CITINGS)

TI Study of artificial flavoring substances for mutagenicity in the  
 SO Salmonella/microsome, Basic and micronucleus tests  
 Food and Chemical Toxicology (1983), 21(6), 707-19  
 CODEN: FCTOD7; ISSN: 0278-6915

AB Seventy-six compds. used as artificial flavoring substances in food  
 products were studied for mutagenic properties by the use of the  
 Salmonella/mammalian microsome test (Ames test), Basic test on *Drosophila*  
*melanogaster*, and micronucleus test on mouse bone marrow. The following 4  
 compds. were mutagenic in Ames tests. EtNO<sub>2</sub> [109-95-5], ethyl  
 3-phenylglycidate [121-39-1], 6-methylquinoline [91-62-3] and musk  
 ambrette. Of these EtNO<sub>2</sub> and musk ambrette also induced an increase in  
 sex-linked recessive lethal mutations in *Drosophila*. Two further compds.  
 ethyl 3-methyl-3-phenylglycidate [77-83-8] and 4-propylanisole  
 [104-45-0], appeared weakly mutagenic in *Drosophila* only. The result with  
 4-propylanisole was of equivocal biol. significance. None of the  
 flavoring substances induced micronuclei, i.e. cytogenetic damage in the  
 bone marrow of mice.

ST flavoring material mutagenicity

IT Mutagens  
 (flavoring materials)

IT Flavoring materials  
 (mutagenicity of)

IT 77-83-8 91-62-3 104-45-0 109-95-5 121-39-1  
 RL: ADV (Adverse effect, including toxicity); FFD (Food or feed use); BIOL  
 (Biological study); USES (Uses)  
 (flavoring material, mutagenicity of)

L29 ANSWER 16 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1983:538318 HCAPLUS

DOCUMENT NUMBER: 99:138318

ORIGINAL REFERENCE NO.: 99:21245a,21248a

TITLE: Volatile flavor components of dried bonito  
 (Katsuobushi). II. From the neutral fraction

AUTHOR(S): Yajima, Izumi; Nakamura, Mikio; Sakakibara, Hidemasa;  
 Ide, Junichi; Yanai, Tetsuya; Hayashi, Kazuo

CORPORATE SOURCE: Kawasaki Res. Lab., T. Hasegawa Co. Ltd., Kawasaki,  
 211, Japan

SOURCE: Agricultural and Biological Chemistry (1983), 47(8),  
 1755-60

CODEN: ABCHA6; ISSN: 0002-1369

DOCUMENT TYPE: Journal

LANGUAGE: English

## ABSTRACT:

The aqueous extract of dried bonito (Katsuobushi) was distilled under reduced  
 pressure.

The resulting distillate was extracted with Et<sub>2</sub>O and the extract was separated into  
 acidic, phenolic, basic, and neutral fractions. The neutral fraction was  
 further fractionated into 10 subfractions by silica gel column chromatog. All  
 these subfractions were analyzed by gas chromatog. and gas chromatog.-mass  
 spectrometry. One hundred and sixty-five compds. were identified and 12  
 compds. were tentatively identified from the neutral fraction. Among them, 111  
 compds. were newly identified as flavor components of Katsuobushi.

TI Volatile flavor components of dried bonito (Katsuobushi). II. From the  
 neutral fraction

SO Agricultural and Biological Chemistry (1983), 47(8), 1755-60

CODEN: ABCHA6; ISSN: 0002-1369

AB . . . were identified and 12 compds. were tentatively identified from  
 the neutral fraction. Among them, 111 compds. were newly identified as  
 flavor components of Katsuobushi.

ST bonito flavor volatile substance  
IT Bonito  
(dried, volatile compds. of, flavor in relation to)  
IT Volatile substances  
Alcohols, biological studies  
Esters, biological studies  
Ethers, biological studies  
Hydrocarbons, biological studies  
Ketones, biological studies  
Lactones  
RL: BIOL (Biological study)  
(of dried bonito, flavor in relation to)  
IT Flavor  
(volatiles, of dried bonito)  
IT 60-12-8 64-17-5, biological studies 66-25-1 71-36-3, biological  
studies 71-41-0, biological studies 76-22-2 77-53-2 78-70-6  
78-92-2 80-71-7 83-33-0 83-34-1 89-71-4 89-74-7 90-12-0  
91-16-7 91-20-3, biological studies 91-57-6 92-52-4, biological  
studies 93-04-9 93-55-0 93-58-3 94-59-7 95-13-6 96-41-3  
98-00-0 98-01-1, biological studies 98-55-5 98-86-2, biological  
studies 100-47-0, biological studies 100-51-6, biological studies  
100-52-7, biological studies 100-84-5 104-45-0 104-55-2  
104-87-0 106-68-3 108-88-3, biological studies 108-94-1, biological  
studies 109-94-4 109-97-7 110-43-0 110-62-3 110-93-0 111-13-7  
111-27-3, biological studies 111-70-6 111-71-7 112-12-9 112-31-2  
112-40-3 112-95-8 120-58-1 120-72-9, biological studies 120-92-3  
122-00-9 122-03-2 122-78-1 123-51-3 124-13-0 124-18-5 124-19-6  
137-32-6 140-29-4 141-78-6, biological studies 271-89-6 470-82-6  
481-34-5 483-76-1 483-77-2 487-12-7 494-99-5 507-70-0 542-54-1  
544-76-3 577-16-2 589-55-9 589-98-0 590-86-3 593-45-3 593-49-7  
600-14-6 616-25-1 623-17-6 626-93-7 629-50-5 629-59-4 629-62-9  
629-78-7 629-80-1 629-92-5 629-94-7 629-97-0 629-99-2 630-01-3  
630-02-4 630-03-5 634-36-6 638-67-5 645-13-6 646-31-1 693-54-9  
706-14-9 821-55-6 928-95-0 930-30-3 930-68-7 1072-83-9  
1120-21-4 1120-72-5 1120-73-6 1121-05-7 1121-18-2 1192-62-7  
1193-18-6 1193-79-9 1197-01-9 1334-76-5 1575-46-8 1576-87-0  
1576-96-1 1679-49-8 1757-42-2 2345-28-0 2548-87-0 2758-18-1  
3131-63-3 3188-00-9 3391-86-4 3796-70-1 4041-11-6 4265-25-2  
4313-02-4 4313-03-5 5337-93-9 5577-44-6 5888-51-7 5888-52-8  
6380-23-0 6443-69-2 6728-26-3 6728-31-0 10547-84-9 13400-02-7  
14963-40-7 18409-17-1 18787-63-8 18829-56-6 23033-96-7  
23048-13-7 25152-83-4 25152-84-5 25586-39-4 26370-28-5  
28790-86-5 29036-25-7 30434-64-1 32142-08-8 33488-51-6  
35389-48-1 38743-20-3 41564-88-9 50306-18-8 56438-71-2  
56722-23-7 57643-02-4 62019-23-2 72692-71-8 79379-60-5  
87259-01-6 87259-53-8 87305-48-4  
RL: BOC (Biological occurrence); BSU (Biological study, unclassified);  
BIOL (Biological study); OCCU (Occurrence)  
(of bonito, flavor in relation to)  
OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD  
(7 CITINGS)  
TI Volatile flavor components of dried bonito (Katsuobushi). II. From the  
neutral fraction  
SO Agricultural and Biological Chemistry (1983), 47(8), 1755-60  
CODEN: ABCHA6; ISSN: 0002-1369  
AB The aqueous extract of dried bonito (Katsuobushi) was distilled under reduced  
pressure. The resulting distillate was extracted with Et2O and the extract was  
separated into acidic, phenolic, basic, and neutral fractions. The neutral  
fraction was further fractionated into 10 subfractions by silica gel  
column chromatog. All these subfractions were analyzed by gas chromatog.  
and gas chromatog.-mass spectrometry. One hundred and sixty-five compds.

were identified and 12 compds. were tentatively identified from the neutral fraction. Among them, 111 compds. were newly identified as flavor components of Katsuoibushi.

ST bonito flavor volatile substance

IT Bonito

(dried, volatile compds. of, flavor in relation to)

IT Volatile substances

Alcohols, biological studies

Esters, biological studies

Ethers, biological studies

Hydrocarbons, biological studies

Ketones, biological studies

Lactones

RL: BIOL (Biological study)

(of dried bonito, flavor in relation to)

IT Flavor

(volatiles, of dried bonito)

IT 60-12-8	64-17-5, biological studies	66-25-1	71-36-3, biological studies
78-92-2	71-41-0, biological studies	76-22-2	77-53-2 78-70-6
91-16-7	80-71-7 83-33-0 83-34-1	89-71-4	89-74-7 90-12-0
93-04-9	91-20-3, biological studies	91-57-6	92-52-4, biological studies
98-00-0	93-55-0 93-58-3	94-59-7	95-13-6 96-41-3
100-52-7,	98-01-1, biological studies	98-55-5	98-86-2, biological studies
104-87-0	100-47-0, biological studies	100-51-6,	biological studies
109-94-4	100-52-7, biological studies	100-84-5	104-45-0 104-55-2
111-27-3,	106-68-3 108-88-3, biological studies	108-94-1,	biological studies
112-40-3	109-97-7 110-43-0	110-62-3	110-93-0 111-13-7
122-00-9	111-70-6 biological studies	111-71-7	112-12-9 112-31-2
137-32-6	112-95-8 120-58-1	120-72-9,	biological studies 120-92-3
481-34-5	122-03-2 122-78-1	123-51-3	124-13-0 124-18-5 124-19-6
544-76-3	140-29-4 141-78-6,	biological studies	271-89-6 470-82-6
600-14-6	483-76-1 483-77-2	487-12-7	494-99-5 507-70-0 542-54-1
629-78-7	577-16-2 589-55-9	589-98-0	590-86-3 593-45-3 593-49-7
630-02-4	616-25-1 623-17-6	626-93-7	629-50-5 629-59-4 629-62-9
706-14-9	629-80-1 629-92-5	629-94-7	629-97-0 629-99-2 630-01-3
1120-21-4	630-03-5 634-36-6	638-67-5	645-13-6 646-31-1 693-54-9
1193-18-6	821-55-6 928-95-0	930-30-3	930-68-7 1072-83-9
1576-96-1	1120-72-5 1120-73-6	1121-05-7	1121-18-2 1192-62-7
3131-63-3	1193-79-9 1197-01-9	1334-76-5	1575-46-8 1576-87-0
4313-02-4	1679-49-8 1757-42-2	2345-28-0	2548-87-0 2758-18-1
6380-23-0	3188-00-9 3391-86-4	3796-70-1	4041-11-6 4265-25-2
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23048-13-7	6443-69-2 6728-26-3	6728-31-0	10547-84-9 13400-02-7
28790-86-5	18409-17-1 18787-63-8	18829-56-6	23033-96-7
35389-48-1	25152-83-4 25152-84-5	25586-39-4	26370-28-5
56722-23-7	29036-25-7 30434-64-1	32142-08-8	33488-51-6
87259-01-6	38743-20-3 41564-88-9	50306-18-8	56438-71-2
	57643-02-4 62019-23-2	72692-71-8	79379-60-5
	87259-53-8 87305-48-4		

RL: BOC (Biological occurrence); BSU (Biological study, unclassified);

BIOL (Biological study); OCCU (Occurrence)

(of bonito, flavor in relation to)

L29 ANSWER 17 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1983:468991 HCAPLUS

DOCUMENT NUMBER: 99:68991

ORIGINAL REFERENCE NO.: 99:10709a,10712a

TITLE: The metabolism of p-propylanisole in the rat and mouse and its variation with dose

AUTHOR(S): Sangster, S. A.; Caldwell, J.; Hutt, A. J.; Smith, R. L.

CORPORATE SOURCE: Dep. Pharmacol., St. Mary's Hosp. Med. Sch., London,  
W2 1PG, UK  
SOURCE: Food and Chemical Toxicology (1983), 21(3), 263-71  
CODEN: FCTOD7; ISSN: 0278-6915  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
ABSTRACT:

The metabolism of the synthetic flavoring, p-propylanisole [104-45-0], was studied in rats and mice and the variation in its metabolism with dose was determined  
[Methoxy-14C]-p-propylanisole was given to female Wistar albino rats orally and male CD-1 mice i.p. at doses ranging from 0.05 to 1500 mg/kg body weight (0.2-20  $\mu$ Ci/animal). The urine, feces, and 14CO<sub>2</sub> in the expired air were collected. The urinary metabolites were separated by solvent extraction, TLC, and high-pressure liquid chromatog., and characterized by mass and NMR spectroscopy and comparison with authentic samples. Three major 14C-labeled urinary metabolites were excreted, 1'- [5349-60-0] and 2'-hydroxy-p-propylanisole [30314-64-8] and p-methoxyhippuric acid [13214-64-7]; 14CO<sub>2</sub> was eliminated in the expired air, arising from oxidative O-demethylation. The relative quantities of the metabolites varied markedly with dose. The percentage of the dose that was O-demethylated fell as the dose increased and the proportion in the form of urinary metabolites increased. The relative proportions of the major urinary metabolites also changed with dose. In view of the great discrepancy between human exposure to p-propylanisole in foods (.apprx.15  $\mu$ g/day) and the doses used for its toxicol. evaluation in animals, these results emphasize the importance of considering dose-dependent metabolism when interpreting the significance for man of animal data obtained at very high doses.

SO Food and Chemical Toxicology (1983), 21(3), 263-71  
CODEN: FCTOD7; ISSN: 0278-6915

AB The metabolism of the synthetic flavoring, p-propylanisole [104-45-0], was studied in rats and mice and the variation in its metabolism with dose was determined [Methoxy-14C]-p-propylanisole was given to. . .  
ST propylanisole flavoring toxicity metab rat  
IT Air, respiratory  
IT Feces  
IT Urine

(p-propylanisole food flavoring metabolites in, toxicity in relation to)  
IT Flavoring materials  
(p-propylanisole, metabolism of, in rats and mice, toxicity in relation to)  
IT 104-45-0

RL: BIOL (Biological study)  
(flavoring material, metabolism of, in rats and mice, toxicity in relation to)

IT 5349-60-0  
RL: BIOL (Biological study)  
(p-propylanisole flavoring material metabolite, in rats and mice, toxicity in relation to)

IT 13214-64-7 30314-64-8  
RL: BIOL (Biological study)  
(p-propylanisole flavoring material metabolite, in rats and mice, toxicity in relation to)

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD  
(1 CITINGS)

SO Food and Chemical Toxicology (1983), 21(3), 263-71  
CODEN: FCTOD7; ISSN: 0278-6915

AB The metabolism of the synthetic flavoring, p-propylanisole [104-45-0], was studied in rats and mice and the variation in its metabolism with dose was determined [Methoxy-14C]-p-propylanisole was given to female Wistar albino rats orally and male CD-1 mice i.p. at doses ranging from 0.05 to 1500

mg/kg body weight (0.2-20  $\mu$ Ci/animal). The urine, feces, and  $^{14}$ C $^{12}$ O $_2$  in the expired air were collected. The urinary metabolites were separated by solvent extraction, TLC, and high-pressure liquid chromatog., and characterized by mass and NMR spectroscopy and comparison with authentic samples. Three major  $^{14}$ C-labeled urinary metabolites were excreted, 1'- [5349-60-0] and 2'-hydroxy-p-propylanisole [30314-64-8] and p-methoxyhippuric acid [13214-64-7];  $^{14}$ C $^{12}$ O $_2$  was eliminated in the expired air, arising from oxidative O-demethylation. The relative quantities of the metabolites varied markedly with dose. The percentage of the dose that was O-demethylated fell as the dose increased and the proportion in the form of urinary metabolites increased. The relative proportions of the major urinary metabolites also changed with dose. In view of the great discrepancy between human exposure to p-propylanisole in foods (.apprx.15  $\mu$ g/day) and the doses used for its toxicol. evaluation in animals, these results emphasize the importance of considering dose-dependent metabolism when interpreting the significance for man of animal data obtained at very high doses.

ST propylanisole flavoring toxicity metab rat

IT Air, respiratory

Feces

Urine

(p-propylanisole food flavoring metabolites in, toxicity in relation to)

IT Flavoring materials

(p-propylanisole, metabolism of, in rats and mice, toxicity in relation to)

IT 104-45-0

RL: BIOL (Biological study)

(flavoring material, metabolism of, in rats and mice, toxicity in relation to)

IT 5349-60-0

RL: BIOL (Biological study)

(p-propylanisole flavoring material metabolite, in rats and mice, toxicity in relation to)

IT 13214-64-7 30314-64-8

RL: BIOL (Biological study)

(p-propylanisole flavoring material metabolite, in rats and mice, toxicity in relation to)

L29 ANSWER 18 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1978:103450 HCAPLUS

DOCUMENT NUMBER: 88:103450

ORIGINAL REFERENCE NO.: 88:16217a,16220a

TITLE: Occurrence of sesquiterpenes in mountain cheese volatiles

AUTHOR(S): Dumont, Jean Pierre; Adda, Jacques

CORPORATE SOURCE: Lab. Technol. Laitiere, Inst. Natl. Rech. Agron., Jouy-en-Josas, Fr.

SOURCE: Journal of Agricultural and Food Chemistry (1978), 26(2), 364-7

CODEN: JAFCAU; ISSN: 0021-8561

DOCUMENT TYPE: Journal

LANGUAGE: English

ABSTRACT:

Gas chromatog.-mass spectrometry of Beaufort cheese volatiles has led to the identification of 140 components including 9 sesquiterpenes. Sesquiterpenes were only found in cheeses made from summer milk when cows were grazing on high-altitude pastures. The effect of the traditional ripening process on volatile flavor compds. is also discussed.

SO Journal of Agricultural and Food Chemistry (1978), 26(2), 364-7

CODEN: JAFCAU; ISSN: 0021-8561

AB . . . made from summer milk when cows were grazing on high-altitude pastures. The effect of the traditional ripening process on volatile flavor compds. is also discussed.

IT Hydrocarbons, biological studies  
Sesquiterpenes and Sesquiterpenoids  
RL: BIOL (Biological study)  
(of cheese flavor)

IT 60-12-8 64-17-5, biological studies 66-25-1 71-23-8, biological studies 71-36-3, biological studies 71-41-0, biological studies 71-43-2, biological studies 74-93-1, biological studies 75-18-3 78-83-1, biological studies 78-92-2 78-93-3, biological studies 83-34-1 91-20-3, biological studies 93-58-3 95-16-9 96-17-3 98-01-1, biological studies 98-82-8 98-85-1 98-86-2, biological studies 100-41-4, biological studies 100-42-5, biological studies 100-51-6, biological studies 100-52-7, biological studies 103-45-7 105-37-3 105-46-4 105-54-4 105-66-8 105-68-0 106-32-1 106-68-3 107-87-9 108-64-5 108-88-3, biological studies 108-95-2, biological studies 109-60-4 110-38-3 110-42-9 110-43-0 110-62-3 110-86-1, biological studies 111-13-7 111-27-3, biological studies 111-65-9, biological studies 111-71-7 111-84-2 111-87-5, biological studies 112-12-9 112-40-3 120-72-9, biological studies 123-51-3 123-66-0 123-86-4 123-92-2 123-96-6 124-13-0 124-18-5 124-19-6 138-86-3 141-78-6, biological studies 151-10-0 473-55-2 505-10-2 513-86-0 543-49-7 556-24-1 565-61-7 590-86-3 591-78-6 593-08-8 624-54-4 624-92-0 626-93-7 628-99-9 629-50-5 629-62-9 644-49-5 693-54-9 705-86-2 706-14-9 713-95-1 819-97-6 821-55-6 1067-20-5 1120-21-4 1319-77-3 1321-94-4 1330-20-7, biological studies 1534-08-3 1618-26-4 1653-30-1 2198-61-0 3268-49-3 3391-86-4 3658-80-8 5870-68-8 6032-29-7 7452-79-1 7783-06-4, biological studies 25429-37-2 25550-14-5 25704-73-8 27936-13-6 28473-21-4 28804-88-8 29224-55-3 29611-84-5 42474-44-2 53535-33-4 61193-19-9 63335-87-5 63335-88-6 65436-56-8  
RL: BIOL (Biological study)  
(of cheese flavor)

OS.CITING REF COUNT: 52 THERE ARE 52 CAPLUS RECORDS THAT CITE THIS RECORD (52 CITINGS)

SO Journal of Agricultural and Food Chemistry (1978), 26(2), 364-7  
CODEN: JAFCAU; ISSN: 0021-8561

AB Gas chromatog.-mass spectrometry of Beaufort cheese volatiles has led to the identification of 140 components including 9 sesquiterpenes. Sesquiterpenes were only found in cheeses made from summer milk when cows were grazing on high-altitude pastures. The effect of the traditional ripening process on volatile flavor compds. is also discussed.

IT Hydrocarbons, biological studies  
Sesquiterpenes and Sesquiterpenoids  
RL: BIOL (Biological study)  
(of cheese flavor)

IT 60-12-8 64-17-5, biological studies 66-25-1 71-23-8, biological studies 71-36-3, biological studies 71-41-0, biological studies 71-43-2, biological studies 74-93-1, biological studies 75-18-3 78-83-1, biological studies 78-92-2 78-93-3, biological studies 83-34-1 91-20-3, biological studies 93-58-3 95-16-9 96-17-3 98-01-1, biological studies 98-82-8 98-85-1 98-86-2, biological studies 100-41-4, biological studies 100-42-5, biological studies 100-51-6, biological studies 100-52-7, biological studies 103-45-7 105-37-3 105-46-4 105-54-4 105-66-8 105-68-0 106-32-1 106-68-3 107-87-9 108-64-5 108-88-3, biological studies 108-95-2, biological studies 109-60-4 110-38-3 110-42-9 110-43-0 110-62-3 110-86-1, biological studies 111-13-7 111-27-3, biological studies 111-65-9, biological studies 111-71-7 111-84-2 111-87-5, biological studies 112-12-9 112-40-3 120-72-9, biological studies 123-51-3 123-66-0

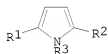
123-86-4 123-92-2 123-96-6 124-13-0 124-18-5 124-19-6 138-86-3  
 141-78-6, biological studies 151-10-0 473-55-2 505-10-2  
 513-86-0 543-49-7 556-24-1 565-61-7 590-86-3 591-78-6 593-08-8  
 624-54-4 624-92-0 626-93-7 628-99-9 629-50-5 629-62-9 644-49-5  
 693-54-9 705-86-2 706-14-9 713-95-1 819-97-6 821-55-6  
 1067-20-5 1120-21-4 1319-77-3 1321-94-4 1330-20-7, biological  
 studies 1534-08-3 1618-26-4 1653-30-1 2198-61-0 3268-49-3  
 3391-86-4 3658-80-8 5870-68-8 6032-29-7 7452-79-1 7783-06-4,  
 biological studies 25429-37-2 25550-14-5 25704-73-8 27936-13-6  
 28473-21-4 28804-88-8 29224-55-3 29611-84-5 42474-44-2  
 53535-33-4 61193-19-9 63335-87-5 63335-88-6 65436-56-8  
 RL: BIOL (Biological study)  
 (of cheese flavor)

L29 ANSWER 19 OF 20 HCAPLUS COPYRIGHT 2011 ACS on SIN

ACCESSION NUMBER: 1976:574492 HCAPLUS  
 DOCUMENT NUMBER: 85:174492  
 ORIGINAL REFERENCE NO.: 85:27889a,27892a  
 TITLE: Heterocyclic flavoring compositions for tobacco  
 INVENTOR(S): Pittet, Alan O.; Pascale, John V.; Hruza, Denis E.  
 PATENT ASSIGNEE(S): International Flavors and Fragrances Inc., USA  
 SOURCE: U.S., 14 pp. Continuation-in-part of U.S. 3,869,554.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3980089	A	19760914	US 1974-468180	19740508 <--
US 3869554	A	19750304	US 1972-246484	19720421 <--
CA 1016737	A1	19770906	CA 1973-163010	19730206 <--
AU 7352088	A	19740815	AU 1973-52088	19730212 <--
CH 566722	A5	19750930	CH 1973-3608	19730313 <--
BE 796761	A1	19730914	BE 1973-128787	19730314 <--
JP 49014668	A	19740208	JP 1973-29552	19730315 <--
FR 2201838	A1	19740503	FR 1973-9410	19730315 <--
GB 1414677	A	19751119	GB 1973-19282	19730424 <--
PRIORITY APPLN. INFO.:			US 1972-246484	A2 19720421

GRAPHIC IMAGE:



# ABSTRACT:

Addition of >1 N-substituted pyrroles (I) (R1 = R2 = H or alkyl; R3 = alkyl, alkenyl, cycloalkyl, phenalkyl, carboalkoxyalkyl, alkoxyphenylalkyl, hydroxyalkyl, alkoxyalkyl, (alkylthio)alkyl, mercaptoalkyl, mercaptophenyl, pyrazinyl, pyridinyl, or thiazolyl) improved the flavor and aroma of tobacco products. Two hundred ml glacial AcOH was added dropwise to a mixture of 2-aminopyrazine 43 and 2,5-dimethoxytetrahydrofuran 66 g at 20°. The mixture was refluxed at 105° for 30 min and, after cooling, was made basic with 325 ml of 30% NaOH and steam-distilled. The distillate was worked up to



obtain 51.3 g N-(2-pyrazinyl)pyrrole (I, R1 = R2 = H, R3 = 2-pyrazinyl) (II). The following mixture was prepared; fenugreek extract 20.00, valerian oil 7.00, dimethylresorcinol 0.25, propylene glycol 39.75, II 3.00, and water 10.00 parts. The mixture, when added to tobacco to 0.10-0.70%, imparted a nutty pyrazinelike odor to the tobacco and conferred a walnut character on the product.

TI Heterocyclic flavoring compositions for tobacco

PI US 3980089 19760914

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3980089	A	19760914	US 1974-468180	19740508 <--
US 3869554	A	19750304	US 1972-246484	19720421 <--
CA 1016737	A1	19770906	CA 1973-163010	19730206 <--
AU 7352088	A	19740815	AU 1973-52088	19730212 <--
CH 566722	A5	19750930	CH 1973-3608	19730313 <--
BE 796761	A1	19730914	BE 1973-128787	19730314 <--
JP 49014668	A	19740208	JP 1973-29552	19730315 <--
FR 2201838	A1	19740503	FR 1973-9410	19730315 <--
GB 1414677	A	19751119	GB 1973-19282	19730424 <--

AB . . . alkyl; R3 = alkyl, alkenyl, cycloalkyl, phenalkyl, carboalkoxyalkyl, alkoxyphenylalkyl, hydroxyalkyl, alkoxyalkyl, (alkylthio)alkyl, mercaptoalkyl, mercaptophenyl, pyrazinyl, pyridinyl, or thiazolyl) improved the flavor and aroma of tobacco products. Two hundred ml glacial AcOH was added dropwise to a mixture of 2-aminopyrazine 43 and. . .

ST tobacco flavor arom compn; pyrrole tobacco flavor aroma; pyrazinylpyrrole tobacco flavor aroma

IT Tobacco

(aroma and flavor of, N-substituted pyrrole improvement of)

IT 57-55-6, biological studies 109-97-7D, 1H-Pyrrole, derivs. 151-10-0

RL: BIOL (Biological study)

(for tobacco aroma and flavor improvement)

IT 5044-41-7P	6719-02-4P	31708-14-2P	50463-83-7P	50966-64-8P
50966-65-9P	50966-66-0P	50966-67-1P	50966-68-2P	50966-70-6P
50966-71-7P	50966-72-8P	50966-73-9P	50966-74-0P	50966-75-1P
50966-76-2P	50966-79-5P			

RL: PREP (Preparation)

(preparation and tobacco aroma and flavor improvement by)

IT 50966-77-3

RL: BIOL (Biological study)

(prep.n. and tobacco aroma and flavor improvement by)

IT 2051-97-0 7435-07-6 23694-49-7

RL: BIOL (Biological study)

(tobacco aroma and flavor improvement by)

OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

TI Heterocyclic flavoring compositions for tobacco

PI US 3980089 19760914

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3980089	A	19760914	US 1974-468180	19740508 <--
US 3869554	A	19750304	US 1972-246484	19720421 <--
CA 1016737	A1	19770906	CA 1973-163010	19730206 <--
AU 7352088	A	19740815	AU 1973-52088	19730212 <--
CH 566722	A5	19750930	CH 1973-3608	19730313 <--
BE 796761	A1	19730914	BE 1973-128787	19730314 <--
JP 49014668	A	19740208	JP 1973-29552	19730315 <--
FR 2201838	A1	19740503	FR 1973-9410	19730315 <--
GB 1414677	A	19751119	GB 1973-19282	19730424 <--

AB Addition of >1 N-substituted pyrroles (I) (R1 = R2 = H or alkyl; R3 = alkyl, alkenyl, cycloalkyl, phenalkyl, carboalkoxyalkyl, alkoxyphenylalkyl, hydroxyalkyl, alkoxyalkyl, (alkylthio)alkyl, mercaptoalkyl, mercaptophenyl, pyrazinyl, pyridinyl, or thiazolyl) improved the flavor and aroma of tobacco products. Two hundred ml glacial AcOH was added dropwise to a mixture of 2-aminopyrazine 43 and 2,5-dimethoxytetrahydrofuran 66 g at 20°. The mixture was refluxed at 105° for 30 min and, after cooling, was made basic with 325 ml of 30% NaOH and steam-distilled. The distillate was worked up to obtain 51.3 g N-(2-pyrazinyl)pyrrole (I, R1 = R2 = H, R3 = 2-pyrazinyl) (II). The following mixture was prepared; fenugreek extract 20.00, valerian oil 7.00, dimethyresorcinol 0.25, propylene glycol 39.75, II 3.00, and water 10.00 parts. The mixture, when added to tobacco to 0.10-0.70%, imparted a nutty pyrazinelike odor to the tobacco and conferred a walnut character on the product.

ST tobacco flavor arom compn; pyrrole tobacco flavor aroma;  
pyrazinylpyrrole tobacco flavor aroma

IT Tobacco  
(aroma and flavor of, N-substituted pyrrole improvement of)

IT 57-55-6, biological studies 109-97-7D, 1H-Pyrrole, derivs.  
151-10-0  
RL: BIOL (Biological study)  
(for tobacco aroma and flavor improvement)

IT 5044-41-7P 6719-02-4P 31708-14-2P 50463-83-7P 50966-64-8P  
50966-65-9P 50966-66-0P 50966-67-1P 50966-68-2P 50966-70-6P  
50966-71-7P 50966-72-8P 50966-73-9P 50966-74-0P 50966-75-1P  
50966-76-2P 50966-79-5P  
RL: PREP (Preparation)  
(preparation and tobacco aroma and flavor improvement by)

IT 50966-77-3  
RL: BIOL (Biological study)  
(prepn. and tobacco aroma and flavor improvement by)

IT 2051-97-0 7435-07-6 23694-49-7  
RL: BIOL (Biological study)  
(tobacco aroma and flavor improvement by)

L29 ANSWER 20 OF 20 HCAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 1976:419413 HCAPLUS  
DOCUMENT NUMBER: 85:19413  
ORIGINAL REFERENCE NO.: 85:3173a,3176a  
TITLE: Flavoring agent  
INVENTOR(S): Winter, Max; Gautschi, Fritz; Flament, Ivon; Stoll, Max; Goldman, Irving M.  
PATENT ASSIGNEE(S): Firmenich S. A., Switz.  
SOURCE: U.S., 8 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 31  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3947603	A	19760330	US 1974-482686	19740624 <--
BR 6679143	D0	19730911	BR 1966-179143	19660429 <--
CH 566111	A5	19750915	CH 1970-13417	19660429 <--
GB 1156487	A	19690625	GB 1966-1156487	19660502 <--
NO 134890	B	19760927	NO 1968-108	19680110 <--
NO 134891	B	19760927	NO 1968-1709	19680502 <--
NO 134892	B	19760927	NO 1968-1710	19680502 <--
NO 134893	B	19760927	NO 1968-1711	19680502 <--
NO 134240	B	19760531	NO 1969-5184	19691231 <--

NO 134894	B	19760927	NO 1969-5180	19691231 <--
NO 134895	B	19760927	NO 1969-5181	19691231 <--
NO 134896	B	19760927	NO 1969-5183	19691231 <--
US 3702253	A	19721107	US 1970-70560	19700908 <--
JP 50004736	B	19750224	JP 1971-19574	19710330 <--
US 4303689	A	19811201	US 1972-243850	19720413 <--
DK 139374	B	19790212	DK 1973-5432	19731005 <--
DK 139374	C	19790716		
DK 139454	B	19790226	DK 1973-5428	19731005 <--
DK 139454	C	19790813		
DK 139553	B	19790312	DK 1973-5429	19731005 <--
DK 139553	C	19790903		
DK 139551	B	19790312	DK 1973-5430	19731005 <--
DK 139551	C	19790903		
DK 139552	B	19790312	DK 1973-5431	19731005 <--
DK 139552	C	19790827		
DK 139605	B	19790319	DK 1973-5426	19731005 <--
DK 139605	C	19790903		
DK 140243	B	19790716	DK 1973-5427	19731005 <--
DK 140243	C	19791203		
DK 140361	B	19790813	DK 1973-5433	19731005 <--
DK 140361	C	19800114		
DK 140362	B	19790813	DK 1973-5434	19731005 <--
DK 140362	C	19800114		
US 3900582	A	19750819	US 1974-482818	19740624 <--
PRIORITY APPLN. INFO.:			US 1965-452342	A2 19650430
			US 1966-543069	A1 19660418
			US 1970-70560	A3 19700908
			US 1972-243866	A3 19720413
			US 1965-542342	A 19650430
			US 1965-543069	A 19650430
			DK 1966-2217	A 19660429
			NO 1966-162820	A 19660429

# ABSTRACT:

Phenolic compds. enhancing or altering the flavor of beverages made from soluble coffee are described. Flavor characteristics in sirup of coffee bases are tabulated for: 2-ethylphenol [90-00-6], 3-ethylphenol [620-17-7], 4-ethylphenol [123-07-9], 4-isopropylphenol [99-89-8], 2,3-xyleneol [526-75-0], 2,4-xyleneol [105-67-9], 2,5-xyleneol [95-87-4], 2,6-xyleneol [576-26-1], 3,4-xyleneol [95-65-8], 3,5-xyleneol [108-68-9], 2-hydroxyacetophenone [582-24-1], 2-hydroxypropiophenone [610-99-1], 4-hydroxypropiophenone [70-70-2], 5-methyl-2-hydroxyacetophenone [1450-72-2], 2,3,5-trimethylphenol [697-82-5], 2,4,6-trimethylphenol [527-60-6], 2,4,5-trimethylphenol [496-78-6], 3,4,5-trimethylphenol [527-54-8], 4-ethyl-2-methoxyphenol [2785-89-9], 4-propyl-2-methoxyphenol [2785-87-7], and 4-vinyl-1,2-dimethoxybenzene [6380-23-0].

## TI Flavoring agent

PI US 3947603 19760330

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	US 3947603	A	19760330	US 1974-482686	19740624 <--
	BR 6679143	D0	19730911	BR 1966-179143	19660429 <--
	CH 566111	A5	19750915	CH 1970-13417	19660429 <--
	GB 1156487	A	19690625	GB 1966-1156487	19660502 <--
	NO 134890	B	19760927	NO 1968-108	19680110 <--
	NO 134891	B	19760927	NO 1968-1709	19680502 <--
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	NO 134893	B	19760927	NO 1968-1711	19680502 <--
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US 3702253	A	19721107	US 1970-70560	19700908 <--											
JP 50004736	B	19750224	JP 1971-19574	19710330 <--											
US 4033689	A	19811201	US 1972-243850	19720413 <--											
DK 139374	B	19790212	DK 1973-5432	19731005 <--											
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DK 139454	B	19790226	DK 1973-5428	19731005 <--											
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DK 139605	B	19790319	DK 1973-5426	19731005 <--											
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DK 140243	B	19790716	DK 1973-5427	19731005 <--											
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DK 140362	C	19800114													
US 3900582	A	19750819	US 1974-482818	19740624 <--											
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ST	coffee flavoring phenolic														
IT	Coffee														
	(flavoring materials for)														
IT	Flavoring materials														
	(for coffee)														
IT	70-70-2	90-00-6	95-65-8	95-87-4	99-89-8	105-67-9	108-68-9								
	123-07-9	496-78-6	526-75-0	527-54-8	527-60-6	576-26-1									
	582-24-1	610-99-1	620-17-7	697-82-5	1450-72-2	2785-87-7									
	2785-89-9	6380-23-0													
	RL: BIOL (Biological study)														
	(flavoring, for coffee)														
OS.	CITING REF COUNT:	2	THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)												
TI	Flavoring agent														
PI	US 3947603 19760330														
	PATENT NO.	KIND	DATE	APPLICATION NO.		DATE									
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PI	US 3947603	A	19760330	US 1974-482686		19740624 <--									
	BR 6679143	D0	19730911	BR 1966-179143		19660429 <--									
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	NO 134891	B	19760927	NO 1968-1709		19680502 <--									
	NO 134892	B	19760927	NO 1968-1710		19680502 <--									
	NO 134893	B	19760927	NO 1968-1711		19680502 <--									

NO 134240	B	19760531	NO 1969-5184	19691231 <--
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US 3702253	A	19721107	US 1970-70560	19700908 <--
JP 50004736	B	19750224	JP 1971-19574	19710330 <--
US 4303689	A	19811201	US 1972-243850	19720413 <--
DK 139374	B	19790212	DK 1973-5432	19731005 <--
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DK 139454	B	19790226	DK 1973-5428	19731005 <--
DK 139454	C	19790813		
DK 139553	B	19790312	DK 1973-5429	19731005 <--
DK 139553	C	19790903		
DK 139551	B	19790312	DK 1973-5430	19731005 <--
DK 139551	C	19790903		
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DK 139552	C	19790827		
DK 139605	B	19790319	DK 1973-5426	19731005 <--
DK 139605	C	19790903		
DK 140243	B	19790716	DK 1973-5427	19731005 <--
DK 140243	C	19791203		
DK 140361	B	19790813	DK 1973-5433	19731005 <--
DK 140361	C	19800114		
DK 140362	B	19790813	DK 1973-5434	19731005 <--
DK 140362	C	19800114		
US 3900582	A	19750819	US 1974-482818	19740624 <--
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ST	coffee flavoring phenolic			
IT	Coffee			
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	123-07-9	496-78-6	526-75-0	527-54-8
	582-24-1	610-99-1	620-17-7	527-60-6
	2785-89-9	6380-23-0	697-82-5	1450-72-2
				2785-87-7
RL:	BIOL (Biological study)			
	(flavoring, for coffee)			